

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:ssspta1617srh

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

\* \* \* \* \* Welcome to STN International \* \* \* \* \*

NEWS 1 Web Page URLs for STN Seminar Schedule - N. America  
NEWS 2 "Ask CAS" for self-help around the clock  
NEWS 3 JAN 27 Source of Registration (SR) information in REGISTRY updated  
and searchable  
NEWS 4 JAN 27 A new search aid, the Company Name Thesaurus, available in  
CA/CAPLUS  
NEWS 5 FEB 05 German (DE) application and patent publication number format  
changes  
NEWS 6 MAR 03 MEDLINE and L MEDLINE reloaded  
NEWS 7 MAR 03 MEDLINE file segment of TOXCENTER reloaded  
NEWS 8 MAR 03 FRANCEPAT now available on STN  
NEWS 9 MAR 29 Pharmaceutical Substances (PS) now available on STN  
NEWS 10 MAR 29 WPIFV now available on STN  
NEWS 11 MAR 29 New monthly current-awareness alert (SDI) frequency in RAPRA  
NEWS 12 APR 26 PROMT: New display field available  
NEWS 13 APR 26 IFIPAT/IFIUDB/IFICDB: New super search and display field  
available  
NEWS 14 APR 26 LITLERT now available on STN  
NEWS 15 APR 27 NLDB: New search and display fields available  
NEWS 16 May 10 PROUSDDR now available on STN  
NEWS 17 May 19 PROUSDDR: One FREE connect hour, per account, in both May  
and June 2004  
NEWS 18 May 12 EXTEND option available in structure searching  
NEWS 19 May 12 Polymer links for the POLYLINK command completed in REGISTRY  
NEWS 20 May 17 FRFULL now available on STN

NEWS EXPRESS MARCH 31 CURRENT WINDOWS VERSION IS V7.00A, CURRENT  
MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),  
AND CURRENT DISCOVER FILE IS DATED 26 APRIL 2004  
NEWS HOURS STN Operating Hours Plus Help Desk Availability  
NEWS INTER General Internet Information  
NEWS LOGIN Welcome Banner and News Items  
NEWS PHONE Direct Dial and Telecommunication Network Access to STN  
NEWS WWW CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that  
specific topic.

All use of STN is subject to the provisions of the STN Customer  
agreement. Please note that this agreement limits use to scientific  
research. Use for software development or design or implementation  
of commercial gateways or other similar uses is prohibited and may  
result in loss of user privileges and other penalties.

\* \* \* \* \* STN Columbus \* \* \* \* \*

FILE 'HOME' ENTERED AT 15:01:15 ON 25 MAY 2004

=> fil reg  
COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
0.21	0.21

FULL ESTIMATED COST

FILE 'REGISTRY' ENTERED AT 15:01:47 ON 25 MAY 2004  
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.  
COPYRIGHT (C) 2004 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file  
provided by InfoChem.

STRUCTURE FILE UPDATES: 24 MAY 2004 HIGHEST RN 685504-43-2  
DICTIONARY FILE UPDATES: 24 MAY 2004 HIGHEST RN 685504-43-2

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

Please note that search-term pricing does apply when  
conducting SmartSELECT searches.

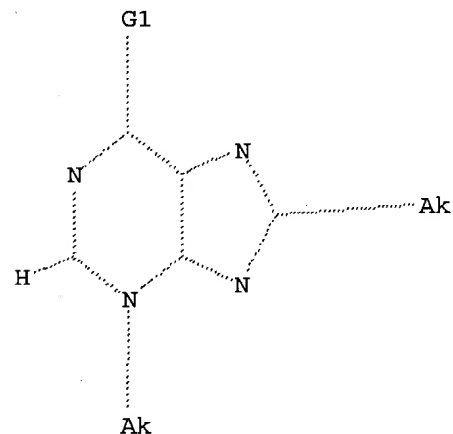
Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more  
information enter HELP PROP at an arrow prompt in the file or refer  
to the file summary sheet on the web at:  
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>  
Uploading C:\Program Files\Stnexp\Queries\hypoxanthine.str

L1 STRUCTURE UPLOADED

=> d  
L1 HAS NO ANSWERS  
L1 STR



G1 O,S

Structure attributes must be viewed using STN Express query preparation.

=> s l1  
SAMPLE SEARCH INITIATED 15:02:42 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 5489 TO ITERATE

18.2% PROCESSED 1000 ITERATIONS

0 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 105339 TO 114221  
PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

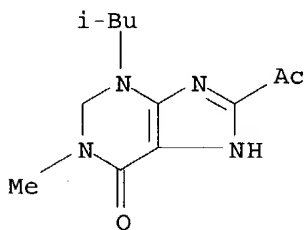
=> s l1 full  
FULL SEARCH INITIATED 15:02:46 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 111306 TO ITERATE

100.0% PROCESSED 111306 ITERATIONS 39 ANSWERS  
SEARCH TIME: 00.00.05

L3 39 SEA SSS FUL L1

=> d scan

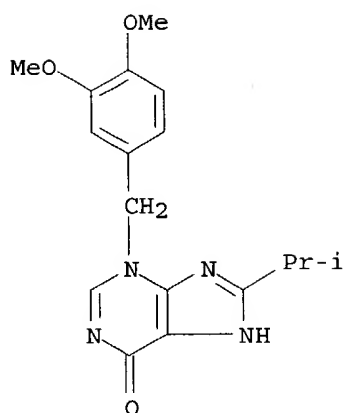
L3 39 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN  
IN 6H-Purin-6-one, 8-acetyl-1,2,3,7-tetrahydro-1-methyl-3-(2-methylpropyl)-  
(9CI)  
MF C12 H18 N4 O2



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

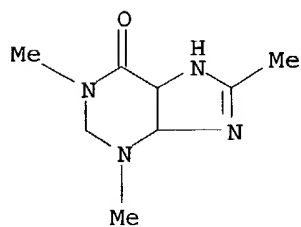
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):38

L3 39 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN  
IN 6H-Purin-6-one, 3-[(3,4-dimethoxyphenyl)methyl]-3,7-dihydro-8-(1-methylethyl)- (9CI)  
MF C17 H20 N4 O3



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

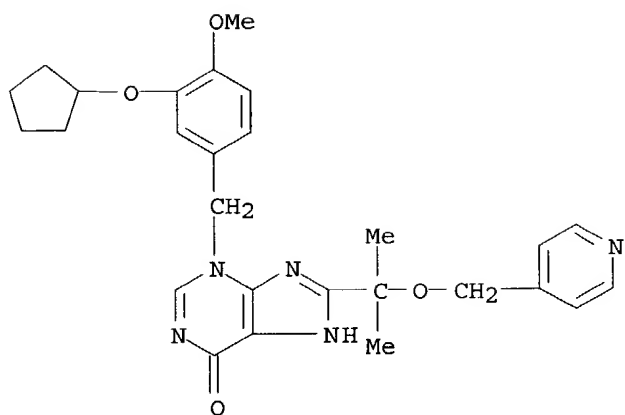
L3 39 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN  
 IN 1H-Purinium, 4,5,6,7-tetrahydro-1,3,8-trimethyl-6-oxo-, iodide (9CI)  
 MF C8 H13 N4 O . I



● I<sup>-</sup>

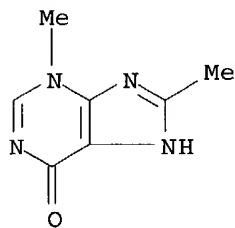
\*\*\* FRAGMENT DIAGRAM IS INCOMPLETE \*\*\*

L3 39 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN  
 IN 6H-Purin-6-one, 3-[[3-(cyclopentyloxy)-4-methoxyphenyl]methyl]-3,7-dihydro-  
 8-[1-methyl-1-(4-pyridinylmethoxy)ethyl]- (9CI)  
 MF C27 H31 N5 O4



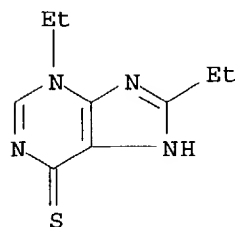
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L3 39 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN  
 IN 6H-Purine-6-one, 3,7-dihydro-3,8-dimethyl- (9CI)  
 MF C7 H8 N4 O



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

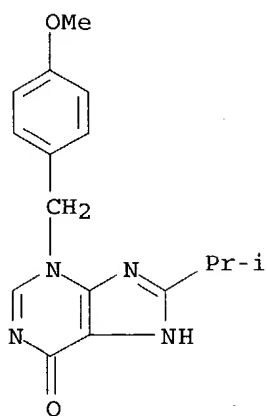
L3 39 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN  
 IN 6H-Purine-6-thione, 3,8-diethyl-3,7-dihydro- (9CI)  
 MF C9 H12 N4 S



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

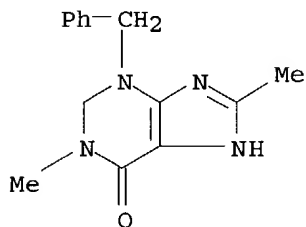
L3 39 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN  
 IN 6H-Purine-6-one, 3,7-dihydro-3-[(4-methoxyphenyl)methyl]-8-(1-methylethyl)- (9CI)

MF C16 H18 N4 O2



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

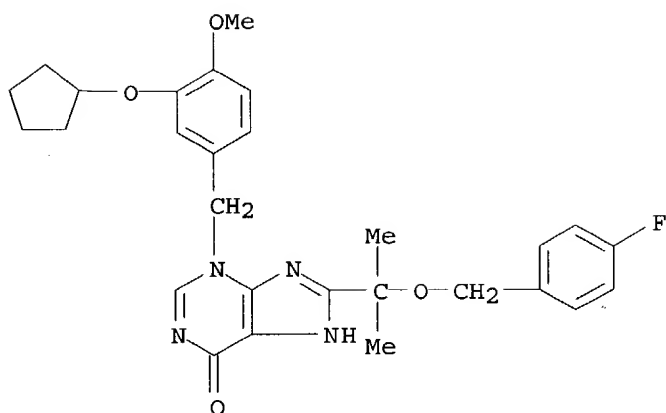
L3 39 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN  
IN 1H-Purinium, 6,7-dihydro-1,8-dimethyl-6-oxo-3-(phenylmethyl)-, iodide  
(9CI)  
MF C14 H15 N4 O . I



● I<sup>-</sup>

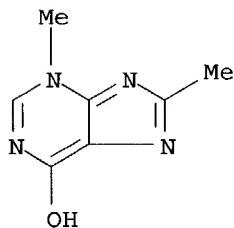
\*\*\* FRAGMENT DIAGRAM IS INCOMPLETE \*\*\*

L3 39 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN  
IN 6H-Purin-6-one, 3-[[3-(cyclopentyloxy)-4-methoxyphenyl]methyl]-8-[1-[(4-fluorophenyl)methoxy]-1-methylethyl]-3,7-dihydro- (9CI)  
MF C28 H31 F N4 O4



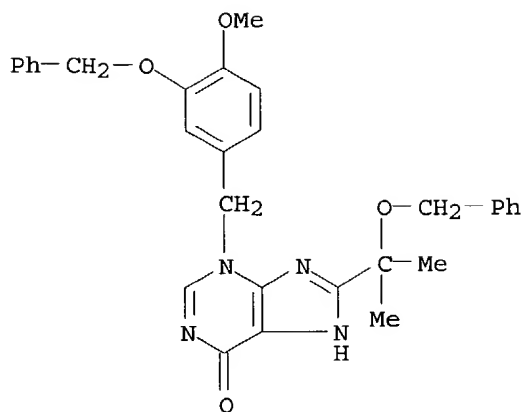
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L3 39 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN  
 IN 3H-Purin-6-ol, 3,8-dimethyl- (9CI)  
 MF C7 H8 N4 O



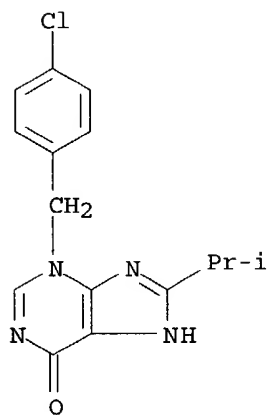
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L3 39 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN  
 IN 6H-Purin-6-one, 3,7-dihydro-3-[[4-methoxy-3-(phenylmethoxy)phenyl]methyl]-  
 8-[1-methyl-1-(phenylmethoxy)ethyl]- (9CI)  
 MF C30 H30 N4 O4



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

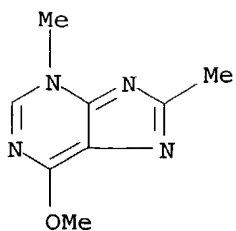
L3 39 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN  
 IN 6H-Purin-6-one, 3-[(4-chlorophenyl)methyl]-3,7-dihydro-8-(1-methylethyl)-  
 (9CI)  
 MF C15 H15 Cl N4 O



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

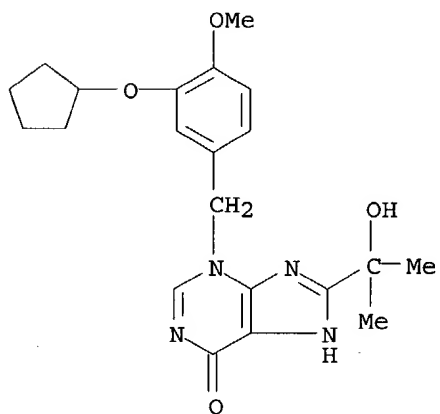
L3 39 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN  
 IN 3H-Purine, 6-methoxy-3,8-dimethyl- (9CI)  
 MF C8 H10 N4 O





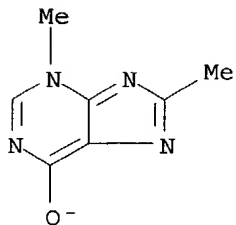
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L3 39 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN  
 IN 6H-Purin-6-one, 3-[[3-(cyclopentyloxy)-4-methoxyphenyl]methyl]-3,7-dihydro-  
 8-(1-hydroxy-1-methylethyl)- (9CI)  
 MF C21 H26 N4 O4



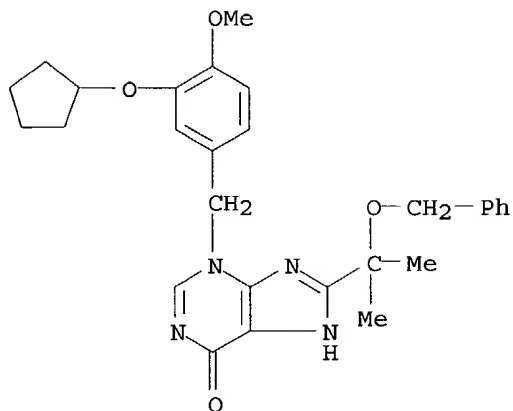
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L3 39 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN  
 IN 3H-Purin-6-ol, 3,8-dimethyl-, ion(1-) (9CI)  
 MF C7 H7 N4 O



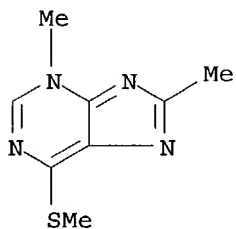
L3 39 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN  
 IN 6H-Purin-6-one, 3-[[3-(cyclopentyloxy)-4-methoxyphenyl]methyl]-3,7-dihydro-  
 8-[1-methyl-1-(phenylmethoxy)ethyl]- (9CI)

MF C28 H32 N4 O4



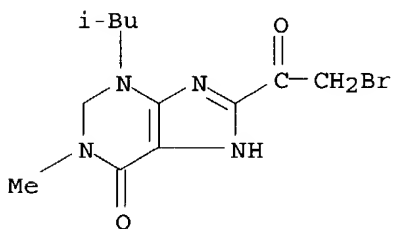
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L3 39 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN  
IN 3H-Purine, 3,8-dimethyl-6-(methylthio)- (7CI, 8CI, 9CI)  
MF C8 H10 N4 S



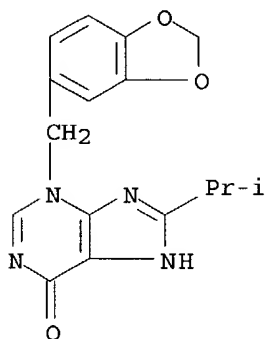
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L3 39 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN  
IN 6H-Purin-6-one, 8-(bromoacetyl)-1,2,3,7-tetrahydro-1-methyl-3-(2-methylpropyl)- (9CI)  
MF C12 H17 Br N4 O2



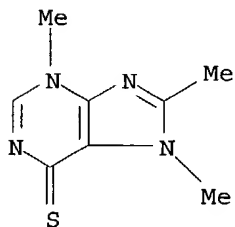
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L3 39 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN  
IN 6H-Purin-6-one, 3-(1,3-benzodioxol-5-ylmethyl)-3,7-dihydro-8-(1-methylethyl)- (9CI)  
MF C16 H16 N4 O3



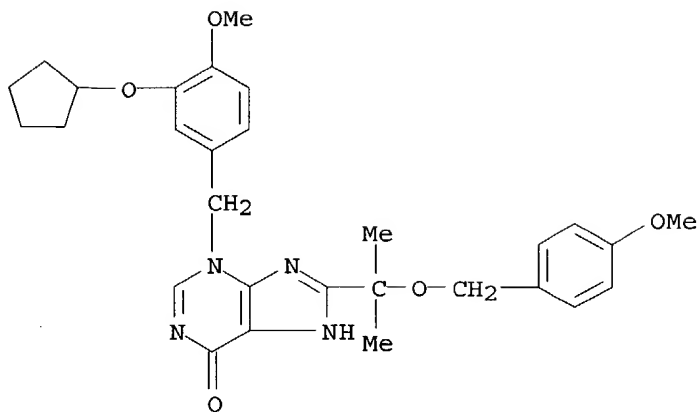
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L3 39 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN  
IN 6H-Purine-6-thione, 3,7-dihydro-3,7,8-trimethyl- (9CI)  
MF C8 H10 N4 S  
CI COM



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

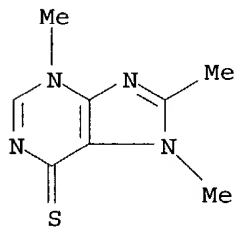
L3 39 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN  
IN 6H-Purin-6-one, 3-[[3-(cyclopentyloxy)-4-methoxyphenyl]methyl]-3,7-dihydro-8-[1-[(4-methoxyphenyl)methoxy]-1-methylethyl]- (9CI)  
MF C29 H34 N4 O5



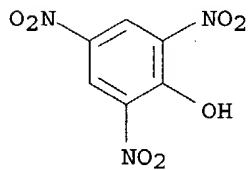
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L3 39 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN  
IN Purine-6(3H)-thione, 3,7,8-trimethyl-, picrate (7CI, 8CI)  
MF C8 H10 N4 S . C6 H3 N3 O7

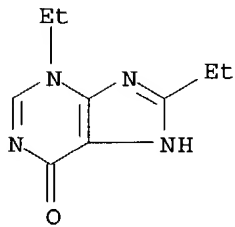
CM 1



CM 2

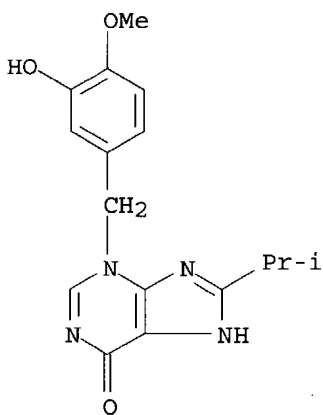


L3 39 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN  
IN 6H-Purin-6-one, 3,8-diethyl-3,7-dihydro- (9CI)  
MF C9 H12 N4 O



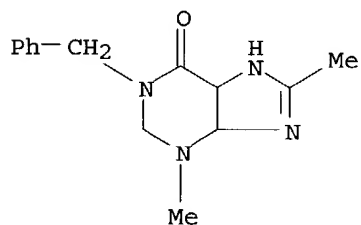
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L3 39 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN  
IN 6H-Purin-6-one, 3,7-dihydro-3-[(3-hydroxy-4-methoxyphenyl)methyl]-8-(1-methylethyl)- (9CI)  
MF C16 H18 N4 O3



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

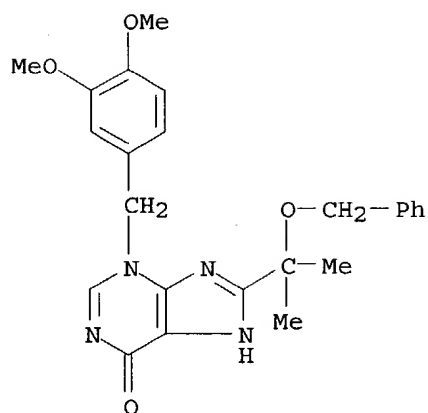
L3 39 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN  
IN 1H-Purinium, 4,5,6,7-tetrahydro-3,8-dimethyl-6-oxo-1-(phenylmethyl)-, bromide (9CI)  
MF C14 H17 N4 O . Br



● Br<sup>-</sup>

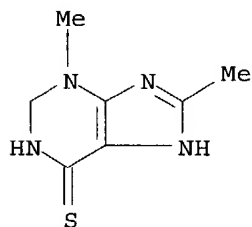
\*\*\* FRAGMENT DIAGRAM IS INCOMPLETE \*\*\*

L3 39 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN  
IN 6H-Purin-6-one, 3-[(3,4-dimethoxyphenyl)methyl]-3,7-dihydro-8-[1-methyl-1-(phenylmethoxy)ethyl]- (9CI)  
MF C24 H26 N4 O4



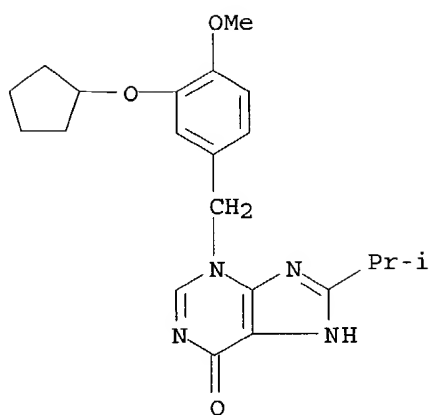
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L3 39 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN  
 IN 6H-Purine-6-thione, 1,2,3,7-tetrahydro-3,8-dimethyl- (9CI)  
 MF C7 H10 N4 S



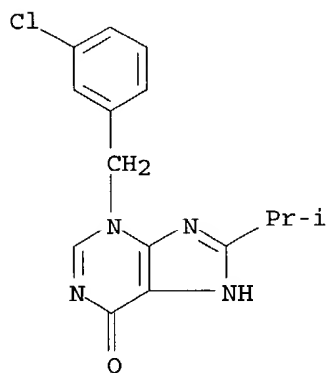
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L3 39 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN  
 IN 6H-Purin-6-one, 3-[[3-(cyclopentyloxy)-4-methoxyphenyl]methyl]-3,7-dihydro-8-(1-methylethyl)- (9CI)  
 MF C21 H26 N4 O3



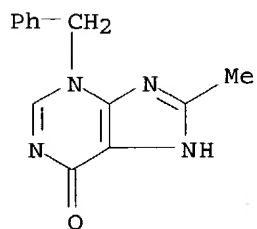
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L3 39 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN  
 IN 6H-Purin-6-one, 3-[(3-chlorophenyl)methyl]-3,7-dihydro-8-(1-methylethyl)-  
 (9CI)  
 MF C15 H15 Cl N4 O



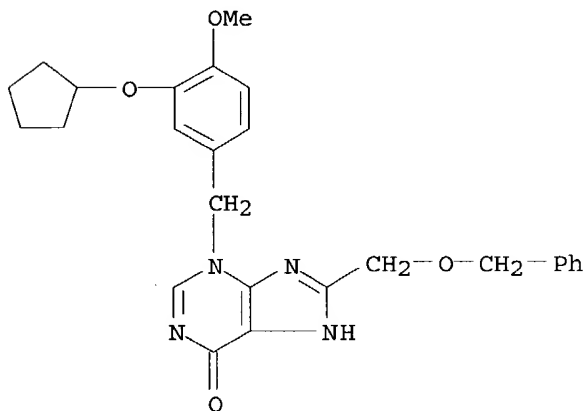
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L3 39 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN  
 IN 6H-Purin-6-one, 3,7-dihydro-8-methyl-3-(phenylmethyl)- (9CI)  
 MF C13 H12 N4 O



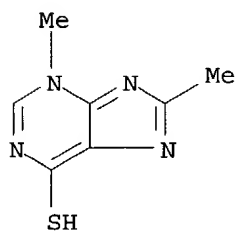
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L3 39 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN  
IN 6H-Purin-6-one, 3-[[3-(cyclopentyloxy)-4-methoxyphenyl]methyl]-3,7-dihydro-  
8-[(phenylmethoxy)methyl]- (9CI)  
MF C26 H28 N4 O4



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

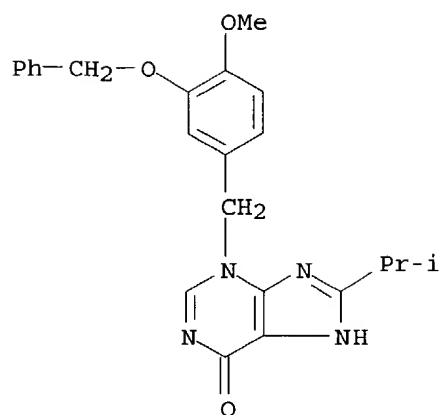
L3 39 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN  
IN 3H-Purine-6-thiol, 3,8-dimethyl- (9CI)  
MF C7 H8 N4 S



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

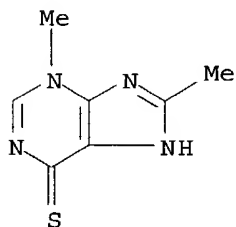
L3 39 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN  
IN 6H-Purin-6-one, 3,7-dihydro-3-[[4-methoxy-3-(phenylmethoxy)phenyl]methyl]-  
8-(1-methylethyl)- (9CI)  
MF C23 H24 N4 O3





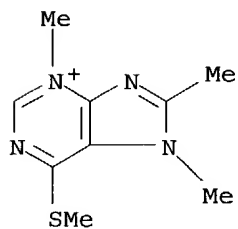
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L3 39 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN  
 IN 6H-Purine-6-thione, 1,3-dihydro-3,8-dimethyl- (9CI)  
 MF C7 H8 N4 S



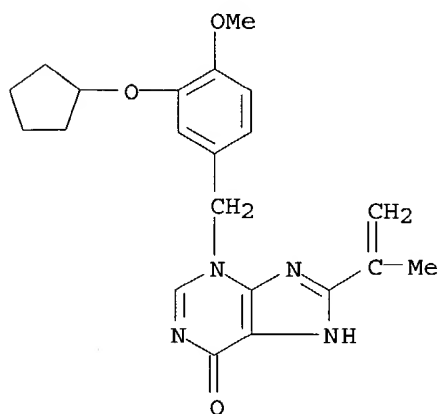
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L3 39 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN  
 IN 3,7,8-Trimethyl-6-(methylthio)purinium iodide (7CI)  
 MF C9 H13 N4 S . I



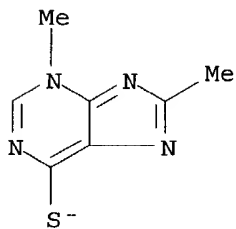
● I<sup>-</sup>

L3 39 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN  
 IN 6H-Purin-6-one, 3-[[3-(cyclopentyloxy)-4-methoxyphenyl]methyl]-3,7-dihydro-  
 8-(1-methylethenyl)- (9CI)  
 MF C21 H24 N4 O3

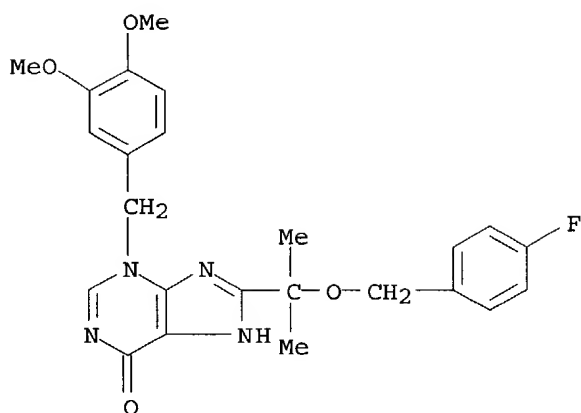


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L3 39 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN  
 IN 3H-Purine-6-thiol, 3,8-dimethyl-, ion(1-) (9CI)  
 MF C7 H7 N4 S

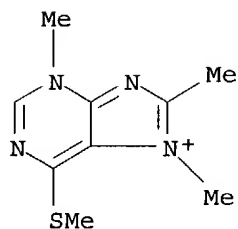


L3 39 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN  
 IN 6H-Purin-6-one, 3-[(3,4-dimethoxyphenyl)methyl]-8-[1-[(4-fluorophenyl)methoxy]-1-methylethyl]-3,7-dihydro- (9CI)  
 MF C24 H25 F N4 O4



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L3 39 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN  
 IN Purinium, 3,7,8-trimethyl-6-(methylthio)-, iodide (8CI)  
 MF C9 H13 N4 S . I



● I<sup>-</sup>

ALL ANSWERS HAVE BEEN SCANNED

=> fil medlin hcapl uspatf wpids  
 COST IN U.S. DOLLARS

FULL ESTIMATED COST

SINCE FILE	TOTAL
ENTRY	SESSION
156.26	156.47

FILE 'MEDLINE' ENTERED AT 15:03:50 ON 25 MAY 2004

FILE 'HCAPLUS' ENTERED AT 15:03:50 ON 25 MAY 2004  
 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
 PLEASE SEE "HELP USAGETERMS" FOR DETAILS.  
 COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)

FILE 'USPATFULL' ENTERED AT 15:03:50 ON 25 MAY 2004  
 CA INDEXING COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)

FILE 'WPIDS' ENTERED AT 15:03:50 ON 25 MAY 2004  
 COPYRIGHT (C) 2004 THOMSON DERWENT

=> s l3  
SAMPLE SEARCH INITIATED 15:03:56 FILE 'WPIDS'  
SAMPLE SCREEN SEARCH COMPLETED - 311 TO ITERATE

100.0% PROCESSED 311 ITERATIONS 3 ANSWERS  
SEARCH TIME: 00.00.07

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 2583 TO 3637  
PROJECTED ANSWERS: 3 TO 81

L4 47 L3

=> dup rem l4  
PROCESSING COMPLETED FOR L4  
L5 46 DUP REM L4 (1 DUPLICATE REMOVED)

=> s l5 not py>1999  
L6 22 L5 NOT PY>1999

=> d ibib abs hitstr 15-22

L6 ANSWER 15 OF 22 USPATFULL on STN  
ACCESSION NUMBER: 1999:96373 USPATFULL  
TITLE: Chemical compounds having PDE-IV inhibition activity  
INVENTOR(S): Cavalla, David, Cambridge, United Kingdom  
Gehrig, Anddre, Basel, Switzerland  
Chasin, Mark, Manalapan, NJ, United States  
Hofer, Peter, Liestal, Switzerland  
Wintergest, Peter, Basel, Switzerland  
PATENT ASSIGNEE(S): Euro-Celtique, S.A., Luxembourg, Luxembourg (non-U.S.  
corporation)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 5939422		19990817
	WO 9500516		19950105
APPLICATION INFO.:	US 1996-578580		19960408 (8)
	WO 1994-GB1334		19940621
			19960408 PCT 371 date
			19960408 PCT 102(e) date

	NUMBER	DATE
PRIORITY INFORMATION:	GB 1993-12853	19930622
DOCUMENT TYPE:	Utility	
FILE SEGMENT:	Granted	
PRIMARY EXAMINER:	Berch, Mark L	
LEGAL REPRESENTATIVE:	Davidson, Davidson & Kappel, LLC	
NUMBER OF CLAIMS:	50	
EXEMPLARY CLAIM:	1,3	
NUMBER OF DRAWINGS:	2 Drawing Figure(s); 2 Drawing Page(s)	
LINE COUNT:	1819	

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB Disclosed is a compound of the formula (I): wherein

R.sub.3, R.sub.6a and R.sub.8 are the same or different and represent a  
C.sub.2-8 alkyl which is unbranched or branched and unsubstituted or  
substituted; C.sub.3-8 cycloalkyl which is unsubstituted or substituted;  
C.sub.4-8 cycloalkylalkyl wherein the cycloalkyl portion is  
unsubstituted or substituted; aryl which is unsubstituted or  
substituted; aralkyl C.sub.1-4 ; heterocyclyl; and heterocyclylalkyl

(C.sub.1 -C.sub.4)

R.sub.6b represents H or R.sub.6a, or together R.sub.6b, N, and R.sub.6a make a C.sub.3 -C.sub.8 ring containing from one to three nitrogen atoms, from zero to two oxygen atoms, from zero to two sulfur atoms, which is optionally substituted;

and where aryl is phenyl or naphthyl, the heterocyclyl is a 5, 6 or 7 membered ring including from one to three nitrogen atoms, and from zero to two oxygen atoms, from zero to two sulfur atoms, and can be substituted as in aryl on the carbons or nitrogens of that ring;

or a pharmaceutically acceptable salt thereof.

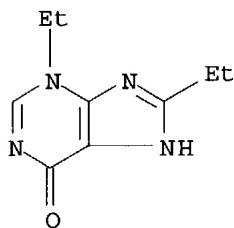
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 162279-42-7P 162279-43-8P

(preparation of purines, isoguanines, and dithioxanthines as phosphodiesterase-IV inhibitors)

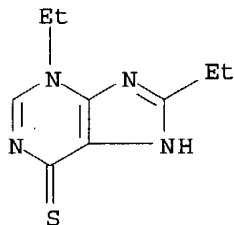
RN 162279-42-7 USPATFULL

CN 6H-Purin-6-one, 3,8-diethyl-3,7-dihydro- (9CI) (CA INDEX NAME)



RN 162279-43-8 USPATFULL

CN 6H-Purine-6-thione, 3,8-diethyl-3,7-dihydro- (9CI) (CA INDEX NAME)



L6 ANSWER 16 OF 22 USPATFULL on STN

ACCESSION NUMBER: 1999:78756 USPATFULL

TITLE: Aryl pyrazole compound for inhibiting phosphodiesterase IV and methods of using same

INVENTOR(S): Cavalla, David John, Cambridge, United Kingdom  
Chasin, Mark, Manalapan, NJ, United States  
Dolby, Lloyd J., Eugene, OR, United States  
Frith, Richard William, Cambridge, United Kingdom

PATENT ASSIGNEE(S): Euro-Celtique, S.A., Luxembourg, Luxembourg (non-U.S. corporation)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 5922751		19990713
APPLICATION INFO.:	US 1997-782502		19970110 (8)
RELATED APPLN. INFO.:	Continuation of Ser. No. US 1995-486184, filed on 7 Jun 1995, now abandoned which is a continuation-in-part of		

Ser. No. US 1994-265641, filed on 24 Jun 1994, now abandoned

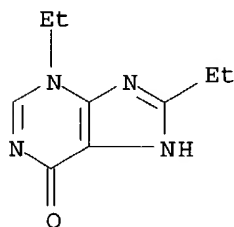
DOCUMENT TYPE: Utility  
FILE SEGMENT: Granted  
PRIMARY EXAMINER: Dees, Jose' G.  
ASSISTANT EXAMINER: Stockton, Laura L.  
LEGAL REPRESENTATIVE: Davidson, Davidson & Kappel, LLC  
NUMBER OF CLAIMS: 24  
EXEMPLARY CLAIM: 1  
LINE COUNT: 1595

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

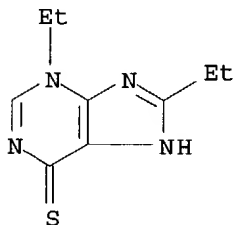
AB Novel compounds which are effective PDE IV inhibitors are disclosed The compounds possess similar or improved PDE IV inhibition as compared to rolipram, with improved selectivity with regard to, e.g., PDE III inhibition. Preferred compounds are 3-(3-cyclopentyloxy-4-methoxybenzylamino)-4-hydroxymethyl pyrazole and 3-(3-cyclopentyloxy-4-methoxybenzylamino)-4-methoxymethylpyrazole.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 162279-42-7P 162279-43-8P  
(preparation of purines, isoguanines, and dithioxanthines as phosphodiesterase-IV inhibitors)  
RN 162279-42-7 USPATFULL  
CN 6H-Purin-6-one, 3,8-diethyl-3,7-dihydro- (9CI) (CA INDEX NAME)



RN 162279-43-8 USPATFULL  
CN 6H-Purine-6-thione, 3,8-diethyl-3,7-dihydro- (9CI) (CA INDEX NAME)



L6 ANSWER 17 OF 22 USPATFULL on STN  
ACCESSION NUMBER: 1999:40431 USPATFULL  
TITLE: Heterocyclic compounds for inhibiting phosphodiesterase IV  
INVENTOR(S): Cavalla, David John, Cambridge, England  
Dolby, Lloyd J., Eugene, OR, United States  
Chasin, Mark, Manalapan, NJ, United States  
PATENT ASSIGNEE(S): Euro-Celtique, S.A., Luxembourg, Luxembourg (non-U.S. corporation)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 5889014		19990330

APPLICATION INFO.: US 1996-716902 19960920 (8)  
RELATED APPLN. INFO.: Division of Ser. No. US 1995-370952, filed on 10 Jan 1995, now patented, Pat. No. US 5591776 which is a continuation-in-part of Ser. No. US 1994-321730, filed on 12 Oct 1994, now patented, Pat. No. US 5665737  
DOCUMENT TYPE: Utility  
FILE SEGMENT: Granted  
PRIMARY EXAMINER: Gupta, Yogendra N.  
LEGAL REPRESENTATIVE: Davidson, Davidson & Kappel, LLC  
NUMBER OF CLAIMS: 16  
EXEMPLARY CLAIM: 1  
LINE COUNT: 914  
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB Novel compounds which are effective PDE IV inhibitors are disclosed. The compounds have the formula: ##STR1## wherein: R.sub.1 and R.sub.2 may be the same or different and each is selected from the group consisting of hydrogen, saturated or unsaturated straight-chain or branched C.sub.1-12 alkyl groups, cycloalkyl and cycloalkyl-alkyl groups containing from 3 to 10 carbon atoms in the cycloalkyl moiety;

R.sub.3 is hydrogen, halogen, or a saturated or unsaturated straight-chain or branched C.sub.1-12 alkyl group, a cycloalkyl and cycloalkyl-alkyl groups containing from 3 to 7 carbon atoms in the cycloalkyl moiety;

R.sub.4 is a phenyl or benzyl or a 6-membered heteroaryl which may be unsubstituted or substituted with one or more halogen atoms, alkyl groups, nitro groups, hydroxyl groups, cyano groups, carboxyl groups, alkoxy group, alkoxycarbonyl, amido, carboxamido, substituted or unsubstituted amino groups, cycloalkyl and cycloalkyl-alkyl groups containing from 3 to 10 carbon atoms in the cycloalkyl moiety, aryl or aralkyl groups preferably containing from about 6 to about 10 carbon atoms, or heterocyclic groups containing nitrogen, oxygen or sulfur in the ring; said alkyl, cycloalkyl, cycloalkyl-alkyl, aryl, and arylalkyl groups being unsubstituted or substituted by halogen atoms, hydroxyl groups, cyano groups, carboxyl groups, alkoxy groups, alkoxycarbonyl, carboxamido or substituted or unsubstituted amino groups, or one or more lower alkyl groups having from 1 to 3 carbon atoms;

Z is selected from the group consisting of --CH.sub.2 CO--, --NHCH.sub.2 --, --CH.sub.2 NH--, --CH.sub.2 CONH--, --CH.sub.2 NHCO--, --CH.sub.2 COCH.sub.2 --, --COCH.sub.2 --, --C(.dbd.NOC(.dbd.O)NHQ)--, and --C(.dbd.NQ)NH--;

X.sub.1 and X.sub.2 may be the same or different and each is O or S;

wherein Q is R.sub.4 or hydrogen except that when Z.dbd.C(.dbd.NOCONHQ)--, R.sub.4 is not benzyl and R.sub.1 and R.sub.2 are both not hydrogen.

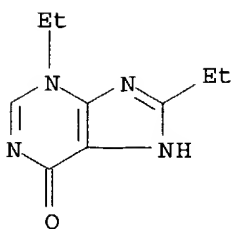
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 162279-42-7P 162279-43-8P

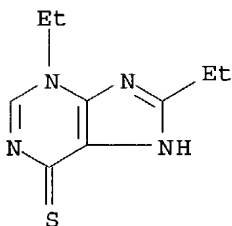
(preparation of purines, isoguanines, and dithioxanthines as phosphodiesterase-IV inhibitors)

RN 162279-42-7 USPATFULL

CN 6H-Purin-6-one, 3,8-diethyl-3,7-dihydro- (9CI) (CA INDEX NAME)



RN 162279-43-8 USPATFULL  
 CN 6H-Purine-6-thione, 3,8-diethyl-3,7-dihydro- (9CI) (CA INDEX NAME)



L6 ANSWER 18 OF 22 USPATFULL on STN  
 ACCESSION NUMBER: 1999:13044 USPATFULL  
 TITLE: Methods for the synthesis of chemical compounds having  
 PDE-IV inhibitory activity  
 INVENTOR(S): Chasin, Mark, Manalapan, NJ, United States  
 Cavalla, David, Cambridge, Great Britain  
 Hofer, Peter, Liestal, Switzerland  
 PATENT ASSIGNEE(S): Euro-Celtique, S.A., Luxembourg, Luxembourg (non-U.S.  
 corporation)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 5864037		19990126
APPLICATION INFO.:	US 1996-659767		19960606 (8)
DOCUMENT TYPE:	Utility		
FILE SEGMENT:	Granted		
PRIMARY EXAMINER:	Berch, Mark L.		
LEGAL REPRESENTATIVE:	Davidson, Davidson & Kappel, LLC		
NUMBER OF CLAIMS:	18		
EXEMPLARY CLAIM:	1		
LINE COUNT:	908		

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB Disclosed is a process for the preparation of a compound of Formula IV  
 having the structure: ##STR1## wherein R.sub.6 is N(R.sub.6a) (R.sub.6b);

R.sub.3 represents a C.sub.2-8, alkyl which is unbranched or branched  
 and unsubstituted or substituted; C.sub.3-8 cycloalkyl which is  
 unsubstituted or substituted; C.sub.4-8 cycloalkylalkyl wherein the  
 cycloalkyl portion is unsubstituted or substituted; aryl or benzyl which  
 is optionally unsubstituted or substituted; ar(C.sub.1-4)alkyl; a  
 heterocyclyl group, ring optionally substituted; heterocyclyl (C.sub.1  
 -C.sub.4) alkyl ring optionally substituted;

which comprises:

- (a) treating a compound of Formula I: ##STR2## with an effective amount  
 of a dethionating agent to produce a compound of Formula II: ##STR3##
- (b) treating a compound of Formula II with an effective halogenating  
 agent under conditions effective to produce a compound of Formula III:



##STR4## and (c) treating a compound of Formula III with an effective aminating agent under conditions effective to produce a compound of Formula IV.

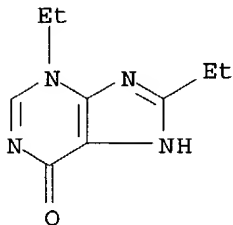
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 162279-42-7P 162279-43-8P

(preparation of purines, isoguanines, and dithioxanthines as phosphodiesterase-IV inhibitors)

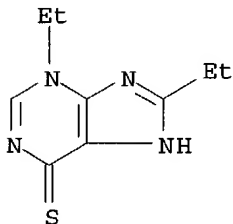
RN 162279-42-7 USPATFULL

CN 6H-Purin-6-one, 3,8-diethyl-3,7-dihydro- (9CI) (CA INDEX NAME)



RN 162279-43-8 USPATFULL

CN 6H-Purine-6-thione, 3,8-diethyl-3,7-dihydro- (9CI) (CA INDEX NAME)



L6 ANSWER 19 OF 22 USPATFULL on STN

ACCESSION NUMBER: 97:81285 USPATFULL

TITLE: Substituted benzoxazoles

INVENTOR(S): Cavalla, John David, Cambridge, England  
Dolby, Lloyd J., Eugene, OR, United States  
Hofer, Peter, Liestal, Switzerland  
Chasin, Mark, Manalapan, NJ, United States

PATENT ASSIGNEE(S): Euro-Celtique, S.A., Luxembourg, Luxembourg (non-U.S. corporation)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 5665737		19970909
APPLICATION INFO.:	US 1994-321730		19941012 (8)
DOCUMENT TYPE:	Utility		
FILE SEGMENT:	Granted		
PRIMARY EXAMINER:	Daus, Donald G.		
LEGAL REPRESENTATIVE:	Steinberg, Raskin & Davidson, P.C.		
NUMBER OF CLAIMS:	24		
EXEMPLARY CLAIM:	1		
LINE COUNT:	986		

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB Novel compounds which are effective PDE IV inhibitors are disclosed. The compounds possess improved PDE IV inhibition as compared to theophylline or rolipram, with improved selectivity with regard to, e.g., PDE III inhibition.

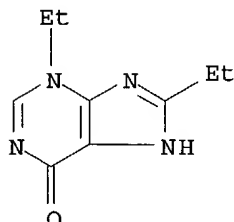
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 162279-42-7P 162279-43-8P

(preparation of purines, isoguanines, and dithioxanthines as  
phosphodiesterase-IV inhibitors)

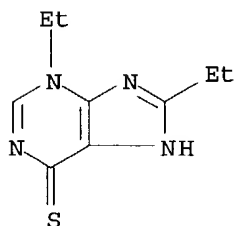
RN 162279-42-7 USPATFULL

CN 6H-Purin-6-one, 3,8-diethyl-3,7-dihydro- (9CI) (CA INDEX NAME)



RN 162279-43-8 USPATFULL

CN 6H-Purine-6-thione, 3,8-diethyl-3,7-dihydro- (9CI) (CA INDEX NAME)



L6 ANSWER 20 OF 22 WPIDS COPYRIGHT 2004 THOMSON DERWENT on STN  
\*\*\*\* DATA NOT AVAILABLE FOR THIS ACCESSION NUMBER

L6 ANSWER 21 OF 22 WPIDS COPYRIGHT 2004 THOMSON DERWENT on STN  
\*\*\*\* DATA NOT AVAILABLE FOR THIS ACCESSION NUMBER

L6 ANSWER 22 OF 22 WPIDS COPYRIGHT 2004 THOMSON DERWENT on STN  
\*\*\*\* DATA NOT AVAILABLE FOR THIS ACCESSION NUMBER

=> fil reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

75.28

231.75

FILE 'REGISTRY' ENTERED AT 15:12:43 ON 25 MAY 2004

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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Property values tagged with IC are from the ZIC/VINITI data file  
provided by InfoChem.

STRUCTURE FILE UPDATES: 24 MAY 2004 HIGHEST RN 685504-43-2

DICTIONARY FILE UPDATES: 24 MAY 2004 HIGHEST RN 685504-43-2

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

Please note that search-term pricing does apply when  
conducting SmartSELECT searches.

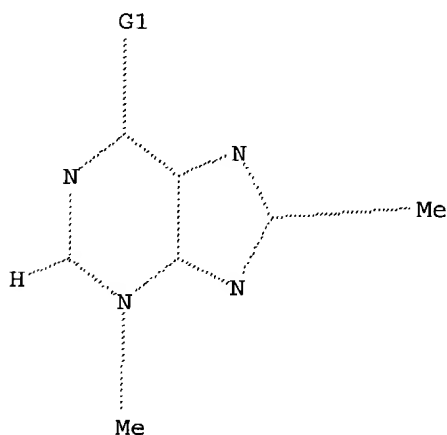
Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:  
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>  
Uploading C:\Program Files\Stnexp\Queries\3,8-dimethyl- hypoxanthine.str

L7 STRUCTURE UPLOADED

=> d  
L7 HAS NO ANSWERS  
L7 STR



G1 O,S

Structure attributes must be viewed using STN Express query preparation.

=> s 17  
SAMPLE SEARCH INITIATED 15:13:08 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 432 TO ITERATE

100.0% PROCESSED 432 ITERATIONS 0 ANSWERS  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 7393 TO 9887  
PROJECTED ANSWERS: 0 TO 0

L8 0 SEA SSS SAM L7

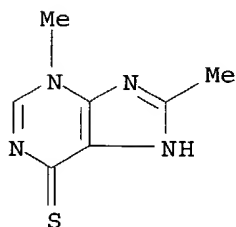
=> s 17 full  
FULL SEARCH INITIATED 15:13:12 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 8709 TO ITERATE

100.0% PROCESSED 8709 ITERATIONS 15 ANSWERS  
SEARCH TIME: 00.00.01

L9 15 SEA SSS FUL L7

=> d scan

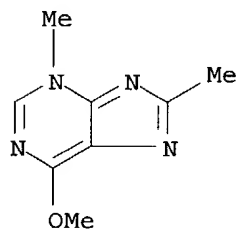
L9 15 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN  
 IN 6H-Purine-6-thione, 1,3-dihydro-3,8-dimethyl- (9CI)  
 MF C7 H8 N4 S



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

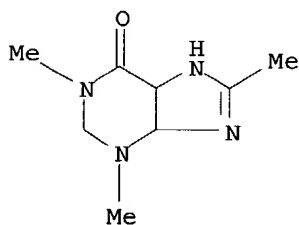
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):14

L9 15 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN  
 IN 3H-Purine, 6-methoxy-3,8-dimethyl- (9CI)  
 MF C8 H10 N4 O



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

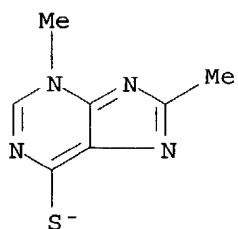
L9 15 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN  
 IN 1H-Purinium, 4,5,6,7-tetrahydro-1,3,8-trimethyl-6-oxo-, iodide (9CI)  
 MF C8 H13 N4 O . I



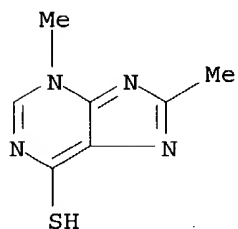
● I<sup>-</sup>

\*\*\* FRAGMENT DIAGRAM IS INCOMPLETE \*\*\*

L9 15 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN  
 IN 3H-Purine-6-thiol, 3,8-dimethyl-, ion(1-) (9CI)  
 MF C7 H7 N4 S

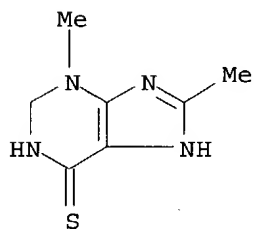


L9 15 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN  
 IN 3H-Purine-6-thiol, 3,8-dimethyl- (9CI)  
 MF C7 H8 N4 S



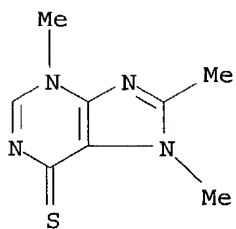
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L9 15 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN  
 IN 6H-Purine-6-thione, 1,2,3,7-tetrahydro-3,8-dimethyl- (9CI)  
 MF C7 H10 N4 S

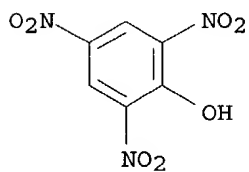


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

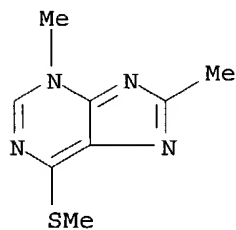
L9 15 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN  
 IN Purine-6(3H)-thione, 3,7,8-trimethyl-, picrate (7CI, 8CI)  
 MF C8 H10 N4 S . C6 H3 N3 O7



CM 2

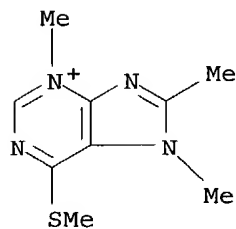


L9 15 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN  
 IN 3H-Purine, 3,8-dimethyl-6-(methylthio)- (7CI, 8CI, 9CI)  
 MF C8 H10 N4 S



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

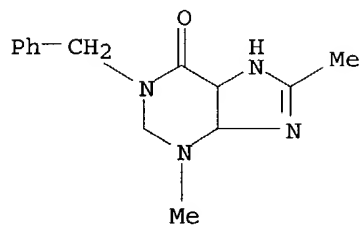
L9 15 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN  
 IN 3,7,8-Trimethyl-6-(methylthio)purinium iodide (7CI)  
 MF C9 H13 N4 S . I



● I<sup>-</sup>

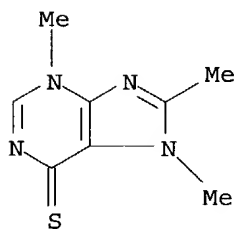
L9 15 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN

IN 1H-Purinium, 4,5,6,7-tetrahydro-3,8-dimethyl-6-oxo-1-(phenylmethyl)-,  
bromide (9CI)  
MF C14 H17 N4 O . Br



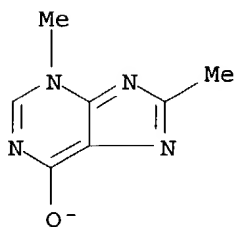
\*\*\* FRAGMENT DIAGRAM IS INCOMPLETE \*\*\*

L9 15 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN  
IN 6H-Purine-6-thione, 3,7-dihydro-3,7,8-trimethyl- (9CI)  
MF C8 H10 N4 S  
CI COM



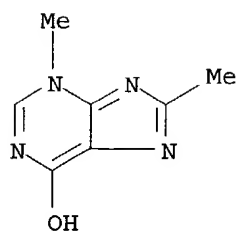
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L9 15 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN  
IN 3H-Purin-6-ol, 3,8-dimethyl-, ion(1-) (9CI)  
MF C7 H7 N4 O



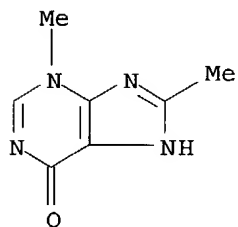
L9 15 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN  
IN 3H-Purin-6-ol, 3,8-dimethyl- (9CI)

MF C7 H8 N4 O



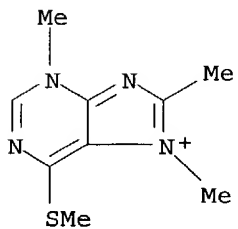
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L9 15 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN  
IN 6H-Purin-6-one, 3,7-dihydro-3,8-dimethyl- (9CI)  
MF C7 H8 N4 O



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L9 15 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN  
IN Purinium, 3,7,8-trimethyl-6-(methylthio)-, iodide (8CI)  
MF C9 H13 N4 S . I



● I<sup>-</sup>

ALL ANSWERS HAVE BEEN SCANNED



=> FIL MEDLIN HCAPL USPATF WPIDS  
COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
155.42	387.17

FULL ESTIMATED COST

FILE 'MEDLINE' ENTERED AT 15:13:35 ON 25 MAY 2004

FILE 'HCAPLUS' ENTERED AT 15:13:35 ON 25 MAY 2004  
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
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FILE 'WPIDS' ENTERED AT 15:13:35 ON 25 MAY 2004  
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=> s 19  
SAMPLE SEARCH INITIATED 15:13:40 FILE 'WPIDS'  
SAMPLE SCREEN SEARCH COMPLETED - 72 TO ITERATE

100.0% PROCESSED 72 ITERATIONS 0 ANSWERS  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 466 TO 974  
PROJECTED ANSWERS: 0 TO 0

L10 12 L9

=> dup rem l10  
PROCESSING COMPLETED FOR L10  
L11 12 DUP REM L10 (0 DUPLICATES REMOVED)

=> d ibib abs hitstr 10-12

L11 ANSWER 10 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1966:104221 HCAPLUS  
DOCUMENT NUMBER: 64:104221  
ORIGINAL REFERENCE NO.: 64:19613b-d  
TITLE: N-Alkylation of 6-methylthiopurines  
AUTHOR(S): Neiman, Z.; Bergmann, F.  
CORPORATE SOURCE: Handassah Med. School, Hebrew Univ., Jerusalem  
SOURCE: Israel J. Chem. (1966), 3(5), 161-72  
DOCUMENT TYPE: Journal  
LANGUAGE: English

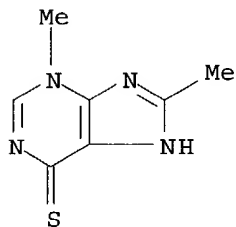
AB N-Methylation was carried out by refluxing 6-methylthiopurines with excess MeI in HCONMe<sub>2</sub> (DMF) or MeCN, removing the solvent in vacuo, and crystallizing the residue. The residue is purified as such or converted to the free base or corresponding betaine. The compound prepared, the refluxing time (hrs.), the solvent used for methylation, and the m.p. of the product were: 3,7-dimethyl-6-methylthio purine iodide (yellow), 1.5, MeCN, 193-4° (decomposition); 3,9-dimethyl-6-methylthiopurine iodide, 2, DMF, 222° (decomposition); 1,9-dimethyl-6-methylthiopurine iodide, 3, DMF, 217-19°; 2,3-dimethyl-6-methylthiopurine, 3, DMF, 192-4°; 3,7,8-trimethyl-6-methylthiopurine iodide, 2, MeCN, 213-14°. For thiohydrolysis, 6-methylthio derivative was dissolved in 10% NH<sub>3</sub>, which had been saturated with H<sub>2</sub>S. After bubbling H<sub>2</sub>S through the solution for an addnl. 10 min., the 6-mercapto derivative was isolated directly or after evaporation to dryness. The yellow 6-mercaptapurines prepared were (substituent and m.p. given): 3,7-dimethyl, 282-3° (H<sub>2</sub>O); 3,9-dimethyl, 276-8°

(AcOH-benzene); 1,9-dimethyl, 250° (AcOH); 2,3-dimethyl, 295-7  
 (AcOH-benzene); 2,3,7-trimethyl, 298-9° (decomposition) (H2O-10% MeCN);  
 3,7,8-trimethyl, 175-8° (decomposition) (EtOH-MeCN). The mechanism of  
 methylation is discussed.

IT 5098-06-6, Purine-6(3H)-thione, 3,8-dimethyl- 5098-10-2,  
 3H-Purine, 3,8-dimethyl-6-(methylthio)- 5759-69-3,  
 Purine-6(3H)-thione, 3,7,8-trimethyl-, picrate  
 (preparation of)

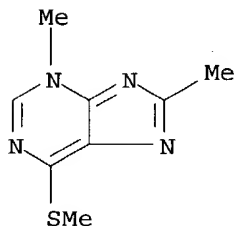
RN 5098-06-6 HCAPLUS

CN 6H-Purine-6-thione, 1,3-dihydro-3,8-dimethyl- (9CI) (CA INDEX NAME)



RN 5098-10-2 HCAPLUS

CN 3H-Purine, 3,8-dimethyl-6-(methylthio)- (7CI, 8CI, 9CI) (CA INDEX NAME)



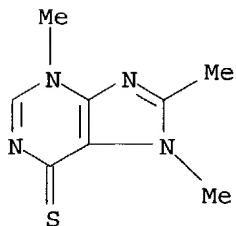
RN 5759-69-3 HCAPLUS

CN Purine-6(3H)-thione, 3,7,8-trimethyl-, picrate (7CI, 8CI) (CA INDEX NAME)

CM 1

CRN 46172-82-1

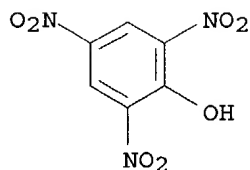
CMF C8 H10 N4 S



CM 2

CRN 88-89-1

CMF C6 H3 N3 O7



L11 ANSWER 11 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1966:11492 HCAPLUS

DOCUMENT NUMBER: 64:11492

ORIGINAL REFERENCE NO.: 64:2087a-d

TITLE: Demethylation of 3-methyl-6-methylthiopurines with hydrogen sulfide

AUTHOR(S): Neiman, Z.; Bergmann, F.

CORPORATE SOURCE: Hebrew Univ.-Hadassah Med. School, Jerusalem

SOURCE: Israel J. Chem. (1965), 3(3), 85-9

DOCUMENT TYPE: Journal

LANGUAGE: English

GI For diagram(s), see printed CA Issue.

AB The title compds., with the quinonoid form of the imidazole ring, readily undergo thiohydrolysis in aqueous solution (I, R = H), (II, R = H), (VII), , (VIII); (III, R = Me), (IV, R = Me), , , ; (V, R = Ph), (VI, R = Ph), , , . Thus, H<sub>2</sub>S bubbled during 20 min. at room temperature through a suspension of I in 25% NH<sub>4</sub>OH and the solution evaporated to dryness in vacuo gives 70% II. Similarly, III gives 60% IV, decomposed 300° (AcOH); V in Me<sub>2</sub>NCHO containing 0.1 volume N NaOH gives VI, decomposed 280-5° (dilute AcOH); and VII gives 80% VIII. 6-Methylthiopurine (non-quinonoid imidazole ring) is unchanged under the same conditions. A mixture of 22 g. 8-phenylhypoxanthine, 100 g. P<sub>2</sub>S<sub>5</sub>, and 500 ml. dry β-picoline was stirred and refluxed 4 hrs., the solvent removed in vacuo, the residue treated 1 hr. with 200 ml. H<sub>2</sub>O at 70°, the insoluble material triturated with 2N NaOH, and the mixture filtered through Celite. The solution was decolorized with C, acidified with AcOH, the precipitate dissolved in 5% Na<sub>2</sub>CO<sub>3</sub>, the solution heated with C, filtered, and cooled. The Na salt which separated was dissolved in hot H<sub>2</sub>O and hot saturated aqueous NH<sub>4</sub>Cl added to give 80%

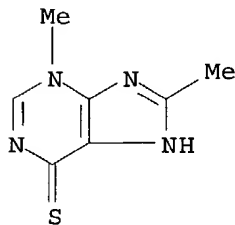
yellow needles of 6-mercapto-8-phenylpurine (IX), decomposed 300°. A solution of 39 g. IX in 600 ml. Me<sub>2</sub>NCHO containing 75 ml. MeI was refluxed 2 hrs., 40 ml. MeI added, reflux continued 2 hrs., and the mixture cooled. The yellow precipitate was dissolved in H<sub>2</sub>O and the pH adjusted to 10 with 2N NaOH to yield 48% V, m. 196-8° (iso-PrOH). Similarly, 6-mercapto-8-methylpurine gave 47% III, m. 195° (MeCN). A solution of 2.5 g. 6-thiotheophylline (VIII) in 15 ml. N NaOH stirred 4 hrs. at room temperature with 2.5 ml. MeI, neutralized with AcOH, evaporated to dryness in

vacuo, and the residue extracted with iso-PrOH gave 22% VII, m. 189-91° (iso-PrOH). Uv and chromatographic data are given.

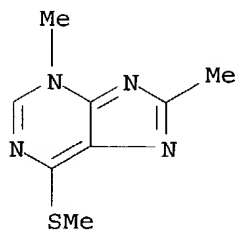
IT 5098-06-6, Purine-6(3H)-thione, 3,8-dimethyl- 5098-10-2, 3H-Purine, 3,8-dimethyl-6-(methylthio)- (preparation of)

RN 5098-06-6 HCAPLUS

CN 6H-Purine-6-thione, 1,3-dihydro-3,8-dimethyl- (9CI) (CA INDEX NAME)



RN 5098-10-2 HCAPLUS  
CN 3H-Purine, 3,8-dimethyl-6-(methylthio)- (7CI, 8CI, 9CI) (CA INDEX NAME)



L11 ANSWER 12 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1962:18329 HCAPLUS  
DOCUMENT NUMBER: 56:18329  
ORIGINAL REFERENCE NO.: 56:3480c-i,3481a-b  
TITLE: Synthesis of 8-substituted purines  
AUTHOR(S): Bergmann, F.; Tamari, M.  
CORPORATE SOURCE: Hebrew Univ., Jerusalem, Israel  
SOURCE: Journal of the Chemical Society, Abstracts (1961)  
4468-72  
CODEN: JCSAAZ; ISSN: 0590-9791  
DOCUMENT TYPE: Journal  
LANGUAGE: Unavailable  
OTHER SOURCE(S): CASREACT 56:18329

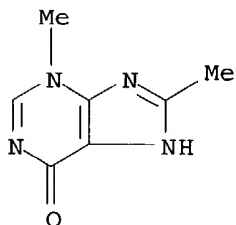
AB Condensation of an acetamidine salt with an appropriate derivative of 4,5-diaminopyrimidine in the absence of a solvent led directly to high yields of the 8-substituted purines (I). General procedure. A mixture of a 4,5-diaminopyrimidine and 2 equivs. MeC(:NH)NH<sub>2</sub>.HCl (II.HCl) heated to 180-90° (homogeneous melt was formed and NH<sub>3</sub> was evolved), when reaction ceased, the melt dissolved in N NaOH, the solution decolorized with C, and acidified with AcOH to pH 6 gave the I, all decomposing above 310° [substituents at 2-, 6-, and 8-position, reaction time in min., % yield, λ (mμ) at pH 8.0, R<sub>f</sub> in 85:10:5 95% EtOH-H<sub>2</sub>OAcOH (solvent A), 70:20:10 95% EtOH-pyridine-H<sub>2</sub>O (solvent B), and 65:25:10 iso-PrOH-HCONMe<sub>2</sub>-10% aqueous NH<sub>3</sub> (solvent C) given]: H, OH, Me, 60, 56 (the yield was improved by addition of 2 equivs. anhydrous NaOAc), 2.52, 0.57, 0.70, --; H, OH, Me, 60, 67 (with II.AcOH), --, --, --, --; OH, OH, Me, 30, 94, 240 and 275, 0.54, 0.60, 0.42; OH, SH, Me (III), 35, 83 (the yield was improved by addition of 2 equivs. anhydrous NaOAc) (the same compound was also prepared in 90% yield from 8-methylxanthine with P<sub>2</sub>S<sub>5</sub>), 251 and 344, 0.50, 0.56, 0.57; SH, OH, Me, 30, 77, 235 and 280, 0.45, 0.74, 0.61; SH, SH, Me, 25, 65 (the yield was improved with 2 equivs. anhydrous NaOAc), 247 and 285, and 351, 0.53, 0.59, 0.71; SH, SH, Me (IV), 25, 86 (with II.AcOH), --, --, --, --; SH, NH<sub>2</sub>, Me (V), 30, 66 (isolated as the sulfate), 230 and 251, and 280, 0.61, 0.67, --; H, OH, Ph, 70, 50, 291, 0.58, 0.79, --; H, OH, Ph, 70, 78 (with II.AcOH), --, --, --; OH, OH, Ph, 40, 80, 228 and 309, 0.52, 0.66, --. Also were prepared 92% 3,8-dimethylxanthine (VI), λ (pH 8.0) 275 m, R<sub>f</sub> 0.64 (in A), 0.79 (in B), and 0.68 (in C), and 88% 3,8-dimethyl-2-mercaptioxanthine (VII), λ (pH 8.0), 233 and 288 mμ, R<sub>f</sub> 0.60 (in A) and 0.84 (in B). N:C(OH).-N:C(NH<sub>2</sub>).C(NH<sub>2</sub>):CH (VIII) (Kalmus and Bergmann, CA 55, 12418h) (1 g.), 1 g. II.HCl, and 0.8 g. anhydrous NaOAc heated 20 min. at 140-5, the resulting cake dissolved in 10% aqueous NH<sub>3</sub>, the solution boiled with C, filtered, and the filtrate kept 24 hrs. in a cold room gave 0.65 g. inseparable mixture of VIII and 2-hydroxy-8-methylpurine (IX), (pH 8.0) 307 m. III (5 g.) and 1.5 g. (wet weight) Raney Ni in 25 ml. 5% aqueous NH<sub>3</sub> refluxed 80 min., filtered, the filtrate adjusted to pH 2 with HNO<sub>3</sub>, and kept 2 months at room temperature gave IX.HNO<sub>3</sub>. If the above ammoniacal solution was acidified with H<sub>2</sub>SO<sub>4</sub>, IX

decomposed quant. The same result was obtained when an ammoniacal solution of IX was evaporated to dryness, the residue extracted with absolute EtOH, and the mixture acidified with 1% alc.-H<sub>2</sub>SO<sub>4</sub>. V (580 mg.) and 1.5 g. (wet weight) Raney Ni in 100 ml. 5% aqueous NH<sub>3</sub> refluxed 2 hrs., filtered hot, and the filtrate cooled gave 300 mg. 8-methyladenine, R<sub>f</sub> 0.57 (in A), 0.67 (in B), and 0.64 (in C). 8-Methylhypoxanthine (1.3 g.), 5 g. P<sub>2</sub>S<sub>5</sub>, and 50 ml. dry pyridine refluxed 4 hrs., concentrated in vacuo, the residue extracted with 37 NaOH, filtered, the solution concentrated in vacuo, and kept overnight at 0° gave 1.1 g. 6-mercapto-8-methylpurine, decomposed above 310° (H<sub>2</sub>O), (pH 8.0) 232 and 316 m, R<sub>f</sub> 0.64 (in A) and 0.71 (in C). VII (1 g.) and 0.7 ml. MeI stirred 30 min. at room temperature in 10 ml. 0.5N NaOH gave 0.95 g. 3,8-dimethyl-2-(methylthio)hypoxanthine, decomposed at 312-15° (H<sub>2</sub>O), R<sub>f</sub> 0.73 (in B). VII (2 g.) and 6 g. (wet weight) Raney Ni in 50 ml. 5% aqueous NH<sub>3</sub> refluxed 2 hrs., filtered, and concentrated in vacuo gave 1.4 g. 3,8-dimethylhypoxanthine, decomposed at 300° (EtOH), R<sub>f</sub> 0.6 (in B). NH.CO.NMe.C(NH<sub>2</sub>):C-(NH<sub>2</sub>).CS (X) and II.HCl or II.AcOH heated at 150-200° gave only X and tars. VI treated with P<sub>2</sub>S<sub>5</sub> in pyridine, concentrated in vacuo, the residue decomposed with cold dilute aqueous NH<sub>3</sub>, the mixture filtered, and the filtrate adjusted to pH 6 with AcOH gave only X, λ (pH 8.0) 249 and 344 mμ, R<sub>f</sub> 0.33 (in A). IV (1 g.) and 2.5 g. Raney Ni in 50 ml. 5% aqueous NH<sub>3</sub> refluxed 70 min., filtered, the filtrate concentrated in vacuo, and kept overnight gave 150 mg. 8-methylpurine, λ (pH 8.0) 266 mμ, R<sub>f</sub> 0.75 (in A).

IT 25108-93-4, Hypoxanthine, 3,8-dimethyl-  
(preparation of)

RN 25108-93-4 HCAPLUS

CN 6H-Purin-6-one, 3,7-dihydro-3,8-dimethyl- (9CI) (CA INDEX NAME)



=> d ibib abs hitstr 1-9

L11 ANSWER 1 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1979:185947 HCAPLUS

DOCUMENT NUMBER: 90:185947

TITLE: Reactivities and electronic aspects of nucleic acid heterocycles. 8. Regioselective radical methylation of carbon-2 and carbon-8 of 6- and 3,6-substituted purines

AUTHOR(S): Zady, Mona F.; Wong, John L.

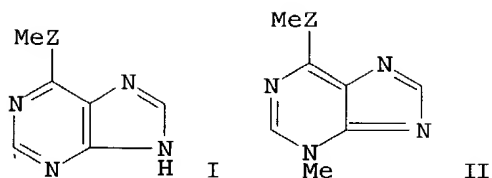
CORPORATE SOURCE: Dep. Chem., Univ. Louisville, Louisville, KY, USA

SOURCE: Journal of Organic Chemistry (1979), 44(9), 1450-4  
CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



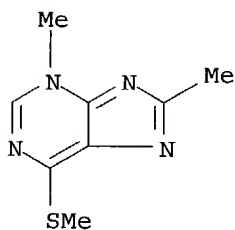
AB Pseudo 1st-order rate consts. were determined for methylation of hypoxanthine, its 3-Me derivative, and I (Z = O,S) and II (Z = O,S) in acidic and neutral media with Me• produced by the photolysis of AcOOCMe<sub>3</sub>. Under acid conditions, hypoxanthine and I yielded mainly 8-methylpurines. 3-Methylhypoxanthine and II were methylated mainly at the 2 position. This regioselectivity was correlated with the site of cation formation via <sup>1</sup>H NMR anal. of the aromatic protons in acidic and neutral media. Methylation occurred fastest at the C atom whose proton resonated at lowest field in the acid NMR spectrum. In neutral solution, the regioselectivity was practically lost in the case of I and reversed to 8-methylation in the case of II. The results are compatible with an SEAr mechanism involving a radical σ complex.

IT 5098-10-2P 25108-93-4P 69257-63-2P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

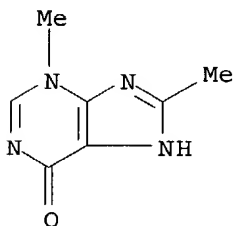
RN 5098-10-2 HCAPLUS

CN 3H-Purine, 3,8-dimethyl-6-(methylthio)- (7CI, 8CI, 9CI) (CA INDEX NAME)



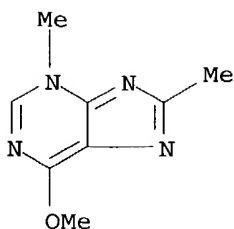
RN 25108-93-4 HCAPLUS

CN 6H-Purin-6-one, 3,7-dihydro-3,8-dimethyl- (9CI) (CA INDEX NAME)



RN 69257-63-2 HCAPLUS

CN 3H-Purine, 6-methoxy-3,8-dimethyl- (9CI) (CA INDEX NAME)



L11 ANSWER 2 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1977:67403 HCAPLUS

DOCUMENT NUMBER: 86:67403

TITLE: Influence of 8-substituents on the oxidation of hypoxanthine and 6-thioxopurine by bovine milk xanthine oxidase

AUTHOR(S): Bergmann, Felix; Levene, Lawrence; Govrin, Hanna; Frank, Aryeh

CORPORATE SOURCE: Hadassah Med. Sch., Hebrew Univ., Jerusalem, Israel  
SOURCE: Biochimica et Biophysica Acta (1977), 480(1), 39-46  
CODEN: BBACAQ; ISSN: 0006-3002

DOCUMENT TYPE: Journal

LANGUAGE: English

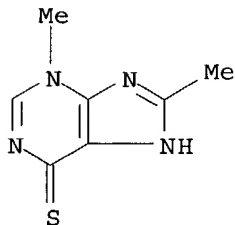
AB The effect of 8-substituents on the rate of oxidation of hypoxanthine and 6-thioxopurine by bovine milk xanthine oxidase was studied. An 8-Me group does not alter the rate of oxidation of hypoxanthine materially, but an 8-Ph substituent reduces it markedly. This is ascribed to inhibition of the tautomerization process, responsible for substrate activation, prior to oxidation. In contrast, the 8-Ph group in 3-methyl-8-phenylhypoxanthine enhances the rate, presumably by binding to a hydrophobic site near the enzymic center. An 8-Ph group in 6-thioxopurine markedly increases the rate of enzymic oxidation. Probably the aromatic substituent diverts anion formation to the imidazole ring. In contrast, ionization of 8-methyl-6-thioxopurine involves the pyrimidine moiety, thus rendering enzymic attack at position 2 more difficult.

IT 5098-06-6 25108-93-4

RL: RCT (Reactant); RACT (Reactant or reagent)  
(oxidation of, kinetics of enzymic)

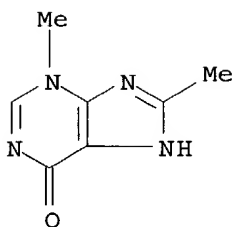
RN 5098-06-6 HCAPLUS

CN 6H-Purine-6-thione, 1,3-dihydro-3,8-dimethyl- (9CI) (CA INDEX NAME)



RN 25108-93-4 HCAPLUS

CN 6H-Purin-6-one, 3,7-dihydro-3,8-dimethyl- (9CI) (CA INDEX NAME)



L11 ANSWER 3 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1976:416151 HCAPLUS

DOCUMENT NUMBER: 85:16151

TITLE: Oxidation of N-methyl substituted hypoxanthines, xanthines, purine-6,8-diones and the corresponding 6-thioxo derivatives by bovine milk xanthine oxidase

AUTHOR(S): Bergmann, Felix; Levene, Lawrence

CORPORATE SOURCE: Hadassah Med. Sch., Hebrew Univ., Jerusalem, Israel

SOURCE: Biochimica et Biophysica Acta (1976), 429(3), 672-88  
CODEN: BBACAQ; ISSN: 0006-3002

DOCUMENT TYPE: Journal

LANGUAGE: English

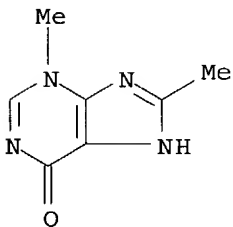
AB The oxidation of 6 series of purines (hypoxanthines, xanthines, purine-6,8-diones, and the corresponding 6-thioxo derivs.) by a highly purified bovine milk xanthine oxidase was studied, using a variety of N-Me derivs. N-Me substituents can either enhance or reduce enzymic rates. Enhancement is ascribed to blockage of groups which mediate unfavorable modes of binding of substrate to enzyme. Introduction of N-Me groups can also inhibit enzymic oxidation, either by occluding essential binding groups or by preventing spontaneous or enzyme-induced tautomerization processes, which create suitable binding sites in the substrates. In all purines which are rapidly attacked by xanthine oxidase, proper attachment to the active center is mediated by the groupings (3)NH, (9)N, or (3)N, (9)NH. Reduced rates usually express lowered substrate affinity, which finds its expression in weak competitive inhibition of xanthine oxidation

IT 25108-93-4

RL: RCT (Reactant); RACT (Reactant or reagent)  
(oxidation of, enzymic)

RN 25108-93-4 HCAPLUS

CN 6H-Purin-6-one, 3,7-dihydro-3,8-dimethyl- (9CI) (CA INDEX NAME)



L11 ANSWER 4 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1976:105543 HCAPLUS

DOCUMENT NUMBER: 84:105543

TITLE: Thermal decomposition of quaternary hypoxanthinium salts and related purines

AUTHOR(S): Bergmann, Felix; Rahat, Miriam

CORPORATE SOURCE: Hadassah Med. Sch., Hebrew Univ., Jerusalem, Israel

SOURCE: Journal of the Chemical Society, Perkin Transactions  
1: Organic and Bio-Organic Chemistry (1972-1999)  
(1976), (2), 239-43



DOCUMENT TYPE:

Journal

LANGUAGE:

English

GI For diagram(s), see printed CA Issue.

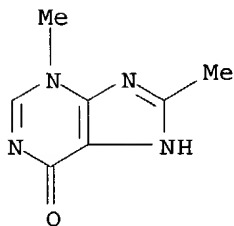
AB Addnl. data considered in abstracting and indexing are available from a source cited in the original document. Thermal decomposition of quaternary hypoxanthinium salts was achieved by heating their solns. in DMF. 1,3-Dialkylhypoxanthinium bromides or iodides lost the 3-substituent as alkyl halide, which then attacked the imidazole ring at N-7 or N-9. Thermolysis of the dioxotetrahydropurinium iodide I (R = H) involved either loss of the 3-Me group as MeI giving the dihydromethylpurinedione II (R = H), or removal of HI to give the corresponding betaine which was then methylated at N-9 to give the dioxotetrahydropurinium iodide I (R = Me). The latter compound in turn decomposed to give the dimethylpurinedione II (R = Me). Similarly, the dimethylhypoxanthinium iodide III (R = H) was degraded mainly by loss of MeI, giving IV (R = H) and small amts. of V (R = H). III (R = H) also lost HI to give the corresponding betaine, which methylated at N-1 to give III (R = Me). III (R = Me) again underwent thermolysis to give a mixture of IV (R = Me) and its 9-Me isomer.

IT 25108-93-4

RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction with Me iodide)

RN 25108-93-4 HCAPLUS

CN 6H-Purin-6-one, 3,7-dihydro-3,8-dimethyl- (9CI) (CA INDEX NAME)

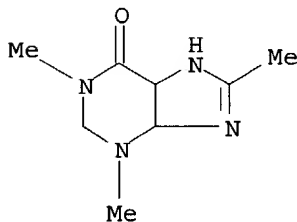


IT 59311-53-4 59311-56-7

RL: RCT (Reactant); RACT (Reactant or reagent)  
(thermal decomposition of)

RN 59311-53-4 HCAPLUS

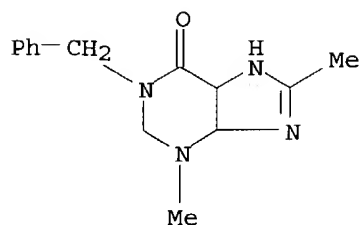
CN 1H-Purinium, 4,5,6,7-tetrahydro-1,3,8-trimethyl-6-oxo-, iodide (9CI) (CA INDEX NAME)

● I<sup>-</sup>

\*\*\* FRAGMENT DIAGRAM IS INCOMPLETE \*\*\*

RN 59311-56-7 HCAPLUS

CN 1H-Purinium, 4,5,6,7-tetrahydro-3,8-dimethyl-6-oxo-1-(phenylmethyl)-, bromide (9CI) (CA INDEX NAME)



● Br<sup>-</sup>

\*\*\* FRAGMENT DIAGRAM IS INCOMPLETE \*\*\*

L11 ANSWER 5 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1973:147123 HCAPLUS

DOCUMENT NUMBER: 78:147123

TITLE: Mechanism of hydrogen-deuterium exchange in hypoxanthines

AUTHOR(S): Lichtenberg, Dov; Bergmann, Felix

CORPORATE SOURCE: Dep. Pharmacol., Heb. Univ., Jerusalem, Israel

SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1973), No. 8, 789-93  
CODEN: JCPRB4; ISSN: 0300-922X

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Kinetic studies on the H-D exchange reactions of 1-, 7-, and 9-methylhypoxanthine and 1,6-, 1,9-, and 7,9-dimethylhypoxanthine showed that the first aromatic proton to undergo exchange was that at C-8. 3-Methyl- and 3,7-dimethylhypoxanthine underwent exchange at C-2 first. Except for 1-methylhypoxanthine the corresponding anions react faster. The exchange proceeded by a protonation-deprotonation mechanism, which for anions involved formation of a zwitterion as the reactive species. Where zwitterion formation was impossible, as in the dianion of hypoxanthine or the monoanion of its 1-Me derivative, the exchange was very slow.

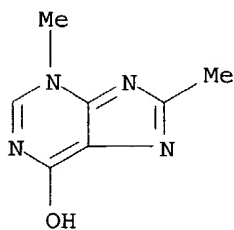
IT 41491-73-0 41491-74-1 41491-76-3

41491-77-4

RL: RCT (Reactant); RACT (Reactant or reagent)  
(exchange reaction of, mechanism and kinetics of)

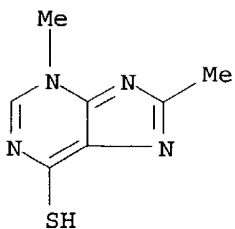
RN 41491-73-0 HCAPLUS

CN 3H-Purin-6-ol, 3,8-dimethyl- (9CI) (CA INDEX NAME)

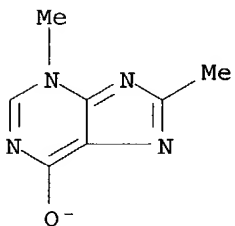


RN 41491-74-1 HCAPLUS

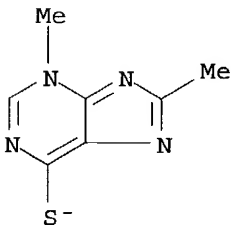
CN 3H-Purine-6-thiol, 3,8-dimethyl- (9CI) (CA INDEX NAME)



RN 41491-76-3 HCAPLUS  
 CN 3H-Purin-6-ol, 3,8-dimethyl-, ion(1-) (9CI) (CA INDEX NAME)



RN 41491-77-4 HCAPLUS  
 CN 3H-Purine-6-thiol, 3,8-dimethyl-, ion(1-) (9CI) (CA INDEX NAME)

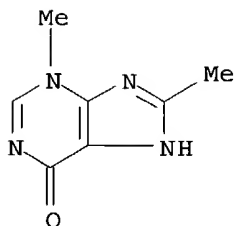


L11 ANSWER 6 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN  
 ACCESSION NUMBER: 1972:474416 HCAPLUS  
 DOCUMENT NUMBER: 77:74416  
 TITLE: Assignment of individual signals of aromatic protons  
 in the NMR spectrum of 6-substituted purines  
 AUTHOR(S): Lichtenberg, D.; Bergmann, F.; Ringel, I.  
 CORPORATE SOURCE: Hadassah Med. Sch., Hebrew Univ., Jerusalem, Israel  
 SOURCE: Journal of Magnetic Resonance (1969-1992) (1972),  
 6(4), 600-4  
 CODEN: JOMRA4; ISSN: 0022-2364  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

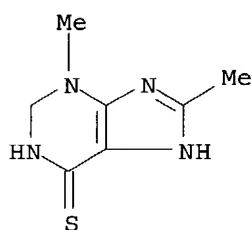
AB Assignment of the resonances of ring protons in substituted purines is  
 made by comparison with the NMR of compds. in which 1 of these protons is  
 substituted by an alkyl group, and by application of the nuclear  
 Overhauser effect to these derivs. in order to identify the signals of  
 protons adjacent to the alkyl substituent. Chemical shifts are given for  
 various ionic forms of the purines in D2O, as well as for the neutral  
 forms.

IT 25108-93-4 38917-32-7  
 RL: PRP (Properties)  
 (NMR of)

RN 25108-93-4 HCAPLUS  
 CN 6H-Purin-6-one, 3,7-dihydro-3,8-dimethyl- (9CI) (CA INDEX NAME)



RN 38917-32-7 HCAPLUS  
 CN 6H-Purine-6-thione, 1,2,3,7-tetrahydro-3,8-dimethyl- (9CI) (CA INDEX NAME)



L11 ANSWER 7 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1971:505114 HCAPLUS

DOCUMENT NUMBER: 75:105114

TITLE: NMR spectra and ionization processes of hypoxanthines

AUTHOR(S): Bergmann, F.; Lichtenberg, D.; Neiman, Z.

CORPORATE SOURCE: Hadassah Med. Sch., Hebrew Univ., Jerusalem, Israel

SOURCE: Quantum Aspects Heterocycl. Compounds Chem. Biochem.,

Proc. Int. Symp., 2nd (1970), Meeting Date 1969,

314-23. Editor(s): Bergmann, Ernst D. Israel Acad.

Sci. Hum.: Jerusalem, Israel.

CODEN: 23ULAG

DOCUMENT TYPE: Conference

LANGUAGE: English

AB The NMR spectra of hypoxanthine and its Me derivative were studied as a 1st approach to solution of the general problem of localization of ionized groups. It was concluded that only a charge in the immediate vicinity of the CH group at positions 2 or 8 influences the chemical shift of its H. Thus, a charge at position 7 or 9 would mainly influence the signal of the H atom on C-8, while ionization processes at one of the N atoms in the pyrimidine ring would mainly shift the band of the H atom on C-2.

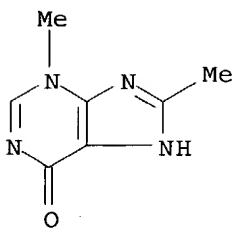
IT 25108-93-4

RL: PROC (Process)

(ionization of, N.M.R. in relation to)

RN 25108-93-4 HCAPLUS

CN 6H-Purin-6-one, 3,7-dihydro-3,8-dimethyl- (9CI) (CA INDEX NAME)

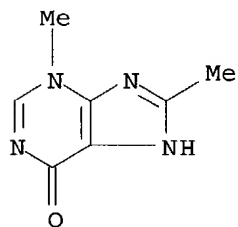


L11 ANSWER 8 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1969:512270 HCAPLUS  
DOCUMENT NUMBER: 71:112270  
TITLE: Hydrogen-deuterium exchange in hypoxanthines  
AUTHOR(S): Bergmann, Felix; Lichtenberg, D.; Neiman, Z.  
CORPORATE SOURCE: Hadassah Med. Sch., Hebrew Univ., Jerusalem, Israel  
SOURCE: Journal of the Chemical Society [Section] D: Chemical  
Communications (1969), (17), 992-3  
CODEN: CCJDAO; ISSN: 0577-6171  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB N.M.R. showed H-D exchange in D2O at 70-85° occurred at position 8 of hypoxanthine and of 7-methyl-, 2-chloro-7-methyl-, and 9-methylhypoxanthine, and at position 2 of 1,8-dimethyl-, 3-methyl-, 3,8-dimethyl-, and 7-methylhypoxanthine. The deuteration was fast at alkaline pH, slow at neutral pH and nil at pH 0. The activation energy for the exchange of 3-methylhypoxanthine was independent of the pH, suggesting the same deuteration mechanism for the neutral and the neg. charged forms.

IT 25108-93-4  
RL: PRP (Properties)  
(exchange of hydrogen with deuterium in)  
RN 25108-93-4 HCAPLUS  
CN 6H-Purin-6-one, 3,7-dihydro-3,8-dimethyl- (9CI) (CA INDEX NAME)



L11 ANSWER 9 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1968:69047 HCAPLUS  
DOCUMENT NUMBER: 68:69047  
TITLE: Preparing 3-methyl-6-thionopurines from  
3-methyl-6-methylthiopurines  
INVENTOR(S): Bergmann, Felix; Neiman, Zohar; Rashi, Moshe  
PATENT ASSIGNEE(S): Yissum Research Development Co.  
SOURCE: Brit., 8 pp.  
CODEN: BRXXAA  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 1073039		19670621		
IL 24642			IL	
PRIORITY APPLN. INFO.:			IL	19651118

GI For diagram(s), see printed CA Issue.

AB The title reaction is effected with H2S in concentrated aqueous NH3. Thus, a mixture

of 22 g. 8-methyl-6-thionopurine, 250 ml. dry HCONMe2 and 30 ml. MeI is refluxed 2 hrs., 15 ml. MeI added, the mixture again refluxed 2 hrs. to give 12 g. Ia (R1 = H, R2 = Me) (I). I (2 g.) is suspended in 50 ml. 25% aqueous NH3 and H2S bubbled through at room temperature for 20 min. to give 1.1 g. Ib (R1 = R2 = H, R3 = Me) decompose 300° (HOAc). Similarly prepared are

Ia (R1 = H, R2 = Ph), m. 196-8° (iso-PrOH) and Ib (R1 = R2 = H, R3 = Ph), decompose 280-5° (dilute HOAc). A solution of 2.5 g. 6-thiotheophylline in 15 ml. N, NaOH is stirred 4 hrs. with 2.5 ml. MeI at room temperature to give 0.6 g. 1,3-dimethyl-6-methylthio-2-oxopurine, m. 189-91° (MeCN), iso-PrOH), which can be converted with H2S/NH3 to 6-thionotheophylline in 80% yield. A solution of 4 g. Ia (R1 = R2 = H) (II) in 80 ml. MeCN is refluxed with 20 ml. MeI for 90 min. to give II.MeI (III), decompose 195-7°; 2 g. III is dissolved in 30 ml. concentrated aqueous NH3 which had been saturated with H2S, H2S bubbled through at room temperature

for

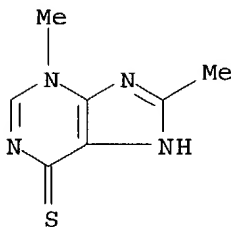
10 min. after which Ib (R1 = R3 = H, R2 = Me), decompose 282-3° (H2O) forms. Also prepared is Ib (R1 = H, R2 = Me, R3 = Ph, m. 242° (HOAc), 4-amino-5-benzamido-6-methylthiopyrimidine, decompose .apprx. 250°; its N-Me analog, m. 214°; 7-methyl-6-methylthio-8-phenylpurine, m. 177°; Ia (R1 = Me, R2 = H), m. 192-4°; Ic (R1 = Me, R2 = R3 = H) decompose 295-7°; Ib (R1 = R2 = Me, R3 = H), decompose 298-9°; 8-(2-pyridyl)hypoxanthine, decompose >300°; 6-thiono-8-(2-pyridyl)purine, decompose >300° (HOAc); Ia (R1 = H, R2 = 2-pyridyl), m. 252°; Ib (R1 = R2 = H, R3 = 2-pyridyl), m. 266°. Details are also provided, for the intermediates and end-products, of  $\lambda_{\text{maximum}}$ ,  $\log \epsilon_{\text{maximum}}$ ,  $R_f$  and color of fluorescence.

IT 5098-06-6P 5098-10-2P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

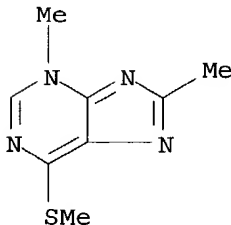
RN 5098-06-6 HCAPLUS

CN 6H-Purine-6-thione, 1,3-dihydro-3,8-dimethyl- (9CI) (CA INDEX NAME)



RN 5098-10-2 HCAPLUS

CN 3H-Purine, 3,8-dimethyl-6-(methylthio)- (7CI, 8CI, 9CI) (CA INDEX NAME)



=> FIL STNGUIDE

COST IN U.S. DOLLARS

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

CA SUBSCRIBER PRICE

SINCE FILE	TOTAL
ENTRY	SESSION
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SINCE FILE	TOTAL
ENTRY	SESSION
-8.32	-8.32

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FILE CONTAINS CURRENT INFORMATION.  
LAST RELOADED: May 21, 2004 (20040521/UP).

=> fil reg		
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CA SUBSCRIBER PRICE	0.00	-8.32

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STRUCTURE FILE UPDATES: 24 MAY 2004 HIGHEST RN 685504-43-2  
DICTIONARY FILE UPDATES: 24 MAY 2004 HIGHEST RN 685504-43-2

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

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Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more  
information enter HELP PROP at an arrow prompt in the file or refer  
to the file summary sheet on the web at:  
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=> fil marpat		
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CA SUBSCRIBER PRICE	0.00	-8.32

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FILE CONTENT: 1988-PRESENT (VOL 140 ISS 21) (20040521/ED)

MOST RECENT CITATIONS FOR PATENTS FROM FIVE MAJOR ISSUING AGENCIES  
(COVERAGE TO THESE DATES IS NOT COMPLETE):

US 6727389 27 APR 2004  
DE 10351214 08 APR 2004  
EP 1406339 07 APR 2004  
JP 2004123716 22 APR 2004  
WO 2004035062 29 APR 2004

Structure search limits have been raised. See HELP SLIMIT for the new, higher limits.

=> s l7

SAMPLE SEARCH INITIATED 15:22:54 FILE 'MARPAT'

SAMPLE SCREEN SEARCH COMPLETED - 160 TO ITERATE

100.0% PROCESSED 160 ITERATIONS

1 ANSWERS

SEARCH TIME: 00.00.02

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 2445 TO 3955

PROJECTED ANSWERS: 1 TO 80

L12 1 SEA SSS SAM L7

=> d

L12 ANSWER 1 OF 1 MARPAT COPYRIGHT 2004 ACS on STN

AN 130:237812 MARPAT

TI Preparation and use of pentopyranosyl-nucleosides

IN Miculka, Christian; Windhab, Norbert; Brandstetter, Tilmann; Burdinski, Gerhard

PA Hoechst A.-G., Germany

SO Ger. Offen., 40 pp.

CODEN: GWXXBX

DT Patent

LA German

FAN.CNT 1

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PI	DE 19741715	A1	19990325	DE 1997-19741715	19970922
	CA 2302414	AA	19990401	CA 1998-2302414	19980921
	CA 2303229	AA	19990401	CA 1998-2303229	19980921
	CA 2303784	AA	19990401	CA 1998-2303784	19980921
	WO 9915539	A2	19990401	WO 1998-EP5997	19980921
	WO 9915539	A3	19990617		
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	RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
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	WO 9915540	A3	19990610		
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	AU 751058	B2	20020808		
	AU 9910245	A1	19990412	AU 1999-10245	19980921
	AU 757983	B2	20030313		
	AU 9910246	A1	19990412	AU 1999-10246	19980921
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	EP 1017703	B1	20040428		
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EP 1019423	B1	20030226		
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BR 9812501	A	20001212	BR 1998-12501	19980921
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JP 2001517676	T2	20011009	JP 2000-512846	19980921
BR 9812381	A	20020430	BR 1998-12381	19980921
AT 233272	E	20030315	AT 1998-950062	19980921
US 6613894	B1	20030902	US 2000-509010	20000320
US 6506896	B1	20030114	US 2000-509039	20000711
US 6608186	B1	20030819	US 2000-509058	20000727
US 2003039997	A1	20030227	US 2002-150402	20020516
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WO 1998-EP5997		19980921		
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US 2000-509039		20000711		

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 For an explanation, enter "HELP SEARCH TYPES"

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FULL ESTIMATED COST	3.11	463.81
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	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-8.32

FILE 'REGISTRY' ENTERED AT 15:25:23 ON 25 MAY 2004  
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STRUCTURE FILE UPDATES: 24 MAY 2004 HIGHEST RN 685504-43-2  
 DICTIONARY FILE UPDATES: 24 MAY 2004 HIGHEST RN 685504-43-2

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

Please note that search-term pricing does apply when  
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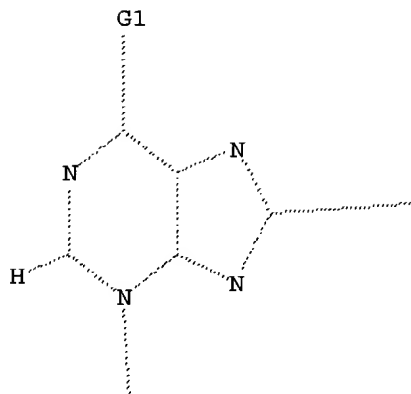
Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more  
 information enter HELP PROP at an arrow prompt in the file or refer  
 to the file summary sheet on the web at:  
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>  
 Uploading C:\Program Files\Stnexp\Queries\hypoxanthine c.str

L13 STRUCTURE UPLOADED

=> d  
 L13 HAS NO ANSWERS  
 L13 STR



G1 O,S

Structure attributes must be viewed using STN Express query preparation.

=> s l13

SAMPLE SEARCH INITIATED 15:25:51 FILE 'REGISTRY'  
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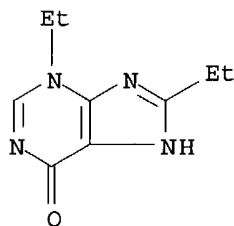
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FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
 BATCH \*\*COMPLETE\*\*  
 PROJECTED ITERATIONS: 7393 TO 9887  
 PROJECTED ANSWERS: 1 TO 80

L14 1 SEA SSS SAM L13

=> d

L14 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2004 ACS on STN  
 RN 162279-42-7 REGISTRY  
 CN 6H-Purin-6-one, 3,8-diethyl-3,7-dihydro- (9CI) (CA INDEX NAME)  
 OTHER NAMES:  
 CN 3,8-Diethylhypoxanthine  
 FS 3D CONCORD  
 MF C9 H12 N4 O  
 SR CA  
 LC STN Files: CA, CAPLUS, USPATFULL  
 DT.CA Caplus document type: Patent  
 RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); RACT  
 (Reactant or reagent); USES (Uses)



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

4 REFERENCES IN FILE CA (1907 TO DATE)  
4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> s l13 full  
FULL SEARCH INITIATED 15:26:06 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 8709 TO ITERATE

100.0% PROCESSED 8709 ITERATIONS 39 ANSWERS  
SEARCH TIME: 00.00.01

L15 39 SEA SSS FUL L13

=> d his

(FILE 'HOME' ENTERED AT 15:01:15 ON 25 MAY 2004)

FILE 'REGISTRY' ENTERED AT 15:01:47 ON 25 MAY 2004

L1 STRUCTURE UPLOADED  
L2 0 S L1  
L3 39 S L1 FULL

FILE 'MEDLINE, HCAPLUS, USPATFULL, WPIDS' ENTERED AT 15:03:50 ON 25 MAY 2004

L4 47 S L3  
L5 46 DUP REM L4 (1 DUPLICATE REMOVED)  
L6 22 S L5 NOT PY>1999

FILE 'REGISTRY' ENTERED AT 15:12:43 ON 25 MAY 2004

L7 STRUCTURE UPLOADED  
L8 0 S L7  
L9 15 S L7 FULL

FILE 'MEDLINE, HCAPLUS, USPATFULL, WPIDS' ENTERED AT 15:13:35 ON 25 MAY 2004

L10 12 S L9  
L11 12 DUP REM L10 (0 DUPLICATES REMOVED)

FILE 'STNGUIDE' ENTERED AT 15:17:39 ON 25 MAY 2004

FILE 'REGISTRY' ENTERED AT 15:22:22 ON 25 MAY 2004

FILE 'MARPAT' ENTERED AT 15:22:28 ON 25 MAY 2004

L12 1 S L7

FILE 'REGISTRY' ENTERED AT 15:25:23 ON 25 MAY 2004

L13 STRUCTURE UPLOADED  
L14 1 S L13  
L15 39 S L13 FULL

=> s l15 not l13

L15 MAY NOT BE USED HERE

The L-number entered was not created by a STRUCTURE or SCREEN command.

=> s l15 not l3

L16 0 L15 NOT L3

=> fil stng

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

157.61

621.42

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-8.32

FILE 'STNGUIDE' ENTERED AT 15:26:43 ON 25 MAY 2004  
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT  
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FILE CONTAINS CURRENT INFORMATION.  
LAST RELOADED: May 21, 2004 (20040521/UP).

=>

---Logging off of STN---

Connection closed by remote host  
END

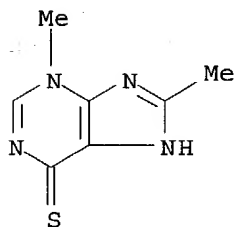
Unable to generate the STN prompt.  
Exiting the script...

ACCESSION NUMBER: 1977:67403 HCAPLUS  
DOCUMENT NUMBER: 86:67403  
TITLE: Influence of 8-substituents on the oxidation of hypoxanthine and 6-thioxopurine by bovine milk xanthine oxidase  
AUTHOR(S): Bergmann, Felix; Levene, Lawrence; Govrin, Hanna; Frank, Aryeh  
CORPORATE SOURCE: Hadassah Med. Sch., Hebrew Univ., Jerusalem, Israel  
SOURCE: Biochimica et Biophysica Acta (1977), 480(1), 39-46  
CODEN: BBACAQ; ISSN: 0006-3002  
DOCUMENT TYPE: Journal  
LANGUAGE: English

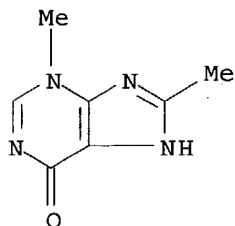
AB The effect of 8-substituents on the rate of oxidation of hypoxanthine and 6-thioxopurine by bovine milk xanthine oxidase was studied. An 8-Me group does not alter the rate of oxidation of hypoxanthine materially, but an 8-Ph substituent reduces it markedly. This is ascribed to inhibition of the tautomerization process, responsible for substrate activation, prior to oxidation. In contrast, the 8-Ph group in 3-methyl-8-phenylhypoxanthine enhances the rate, presumably by binding to a hydrophobic site near the enzymic center. An 8-Ph group in 6-thioxopurine markedly increases the rate of enzymic oxidation. Probably the aromatic substituent diverts anion formation to the imidazole ring. In contrast, ionization of 8-methyl-6-thioxopurine involves the pyrimidine moiety, thus rendering enzymic attack at position 2 more difficult.

IT 5098-06-6 25108-93-4  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(oxidation of, kinetics of enzymic)

RN 5098-06-6 HCAPLUS  
CN 6H-Purine-6-thione, 1,3-dihydro-3,8-dimethyl- (9CI) (CA INDEX NAME)



RN 25108-93-4 HCAPLUS  
CN 6H-Purin-6-one, 3,7-dihydro-3,8-dimethyl- (9CI) (CA INDEX NAME)



L11 ANSWER 3 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1976:416151 HCAPLUS  
DOCUMENT NUMBER: 85:16151  
TITLE: Oxidation of N-methyl substituted hypoxanthines, xanthines, purine-6,8-diones and the corresponding 6-thioxo derivatives by bovine milk xanthine oxidase  
AUTHOR(S): Bergmann, Felix; Levene, Lawrence  
CORPORATE SOURCE: Hadassah Med. Sch., Hebrew Univ., Jerusalem, Israel

SOURCE: Biochimica et Biophysica Acta (1976), 429(3), 672-88  
CODEN: BBACAQ; ISSN: 0006-3002  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB The oxidation of 6 series of purines (hypoxanthines, xanthines, purine-6,8-diones, and the corresponding 6-thioxo derivs.) by a highly purified bovine milk xanthine oxidase was studied, using a variety of N-Me derivs. N-Me substituents can either enhance or reduce enzymic rates. Enhancement is ascribed to blockage of groups which mediate unfavorable modes of binding of substrate to enzyme. Introduction of N-Me groups can also inhibit enzymic oxidation, either by occluding essential binding groups or by preventing spontaneous or enzyme-induced tautomerization processes, which create suitable binding sites in the substrates. In all purines which are rapidly attacked by xanthine oxidase, proper attachment to the active center is mediated by the groupings (3)NH, (9)N, or (3)N, (9)NH. Reduced rates usually express lowered substrate affinity, which finds its expression in weak competitive inhibition of xanthine oxidation

IT 25108-93-4

RL: RCT (Reactant); RACT (Reactant or reagent)  
(oxidation of, enzymic)

RN 25108-93-4 HCAPLUS

CN 6H-Purin-6-one, 3,7-dihydro-3,8-dimethyl- (9CI) (CA INDEX NAME)

